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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:33:00 ON 29 APR 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:33:10 ON 29 APR 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 APR 2008 HIGHEST RN 1017984-01-8
DICTIONARY FILE UPDATES: 28 APR 2008 HIGHEST RN 1017984-01-8

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10813056\rce.str

chain nodes :
7 8 9 10 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :

5-7 7-8 7-9 7-12 8-11 8-13 9-10 9-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-12 8-11 8-13 9-10 9-14
exact bonds :
5-7 7-8 7-9

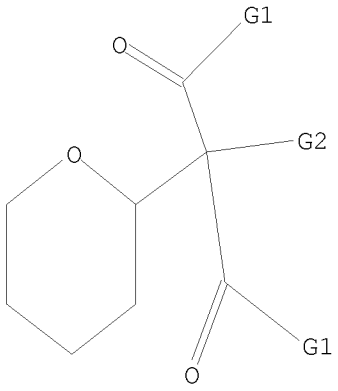
G1:O,N

G2:C,H,Cl,Br,F

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR



G1 O,N
G2 C,H,Cl,Br,F

Structure attributes must be viewed using STN Express query preparation.

=> s l
L2   2355975 L

=> s l1
SAMPLE SEARCH INITIATED 08:33:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   373 TO ITERATE

100.0% PROCESSED   373 ITERATIONS   8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 6302 TO   8618
PROJECTED ANSWERS: 8 TO   329

```
L3            8 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 08:33:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     7696 TO ITERATE

100.0% PROCESSED     7696 ITERATIONS                              133 ANSWERS
SEARCH TIME: 00.00.01

L4          133 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  183.51     183.72

FILE 'CAPLUS' ENTERED AT 08:33:43 ON 29 APR 2008
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FILE LAST UPDATED: 28 Apr 2008  (20080428/ED)

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=> s l4
L5            65 L4

=> s l5 and py<=2003
      23980412 PY<=2003
L6            60 L5 AND PY<=2003

=> d l6 1-60 ibib abs hitstr

L6   ANSWER 1 OF 60  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2003:901818  CAPLUS
DOCUMENT NUMBER:          140:199515
TITLE:                    Carbohydrate-protein interactions at interfaces:
                          comparison of the binding of Ricinus communis lectin
                          to two series of synthetic glycolipids using surface
                          plasmon resonance studies
AUTHOR(S):                Critchley, P.; Clarkson, G. J.
CORPORATE SOURCE:         Department of Chemistry, University of Warwick,
                          Coventry, CV4 7AL, UK
```

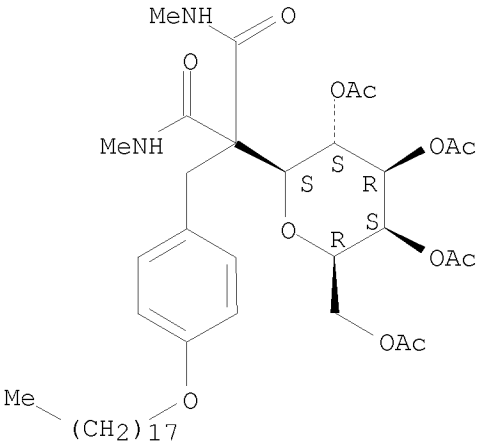
SOURCE: Organic & Biomolecular Chemistry (2003), 1(23), 4148-4159
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:199515

AB Two C-lactosyl lipids and the related C-galactosyl lipids have been synthesized and their binding to RCA120 plant lectin was compared with a second series of thiolactosylethoxyalkanes. The interactions were measured quant. in real time by surface plasmon resonance (BIAcore) at a range of concns. and temps. from 5 to 30 °C. The C-galactosyl lipid (1,3-dimethyl-5-[β-d-galactopyranosyl]-5-(4-octadecyloxybenzyl)pyrimidine-2,4,6-trione) bound much more weakly with a KA = 8.86 + 105 than the corresponding C-lactosyl lipid (1,3-dimethyl-5-[β-d-galactopyranosyl-(1 4)-β-d-glucopyranosyl]-5-(4-octadecyloxybenzyl)pyrimidine-2,4,6-trione) (KA = 2.31 + 107). The influence of the linker region of the two different series of lactosyl lipids was clearly demonstrated by the differences in the binding to RCA120 lectin. The changes in kinetic values and in the enthalpic and entropic contribution to the free energy of binding reflected the importance of the linker and the hydrocarbon anchor holding the synthetic glycolipids in the neomembrane.

IT 660850-45-3P 660850-46-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(comparison of the binding of Ricinus communis lectin to synthetic glycolipids using surface plasmon resonance studies)

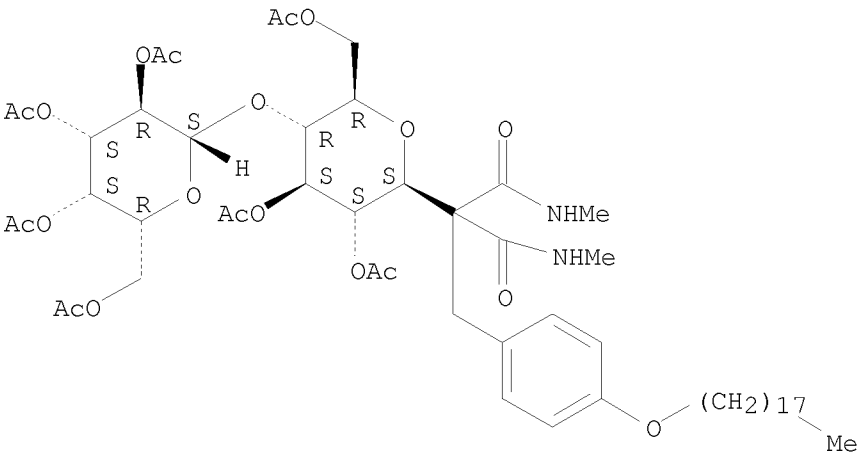
RN 660850-45-3 CAPLUS
CN Propanediamide, N,N'-dimethyl-2-[[4-(octadecyloxy)phenyl]methyl]-2-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 660850-46-4 CAPLUS
CN Propanediamide, N,N'-dimethyl-2-[[4-(octadecyloxy)phenyl]methyl]-2-[2,3,6-tri-O-acetyl-4-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]- (9CI) (CA INDEX NAME)

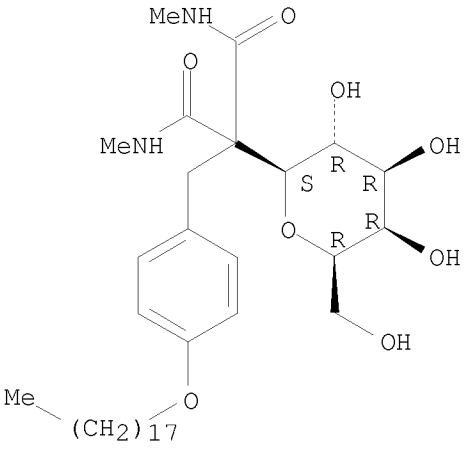
Absolute stereochemistry.



IT 660850-39-5P 660850-40-8P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, acetylation and binding kinetics of; comparison of the binding of Ricinus communis lectin to synthetic glycolipids using surface plasmon resonance studies)

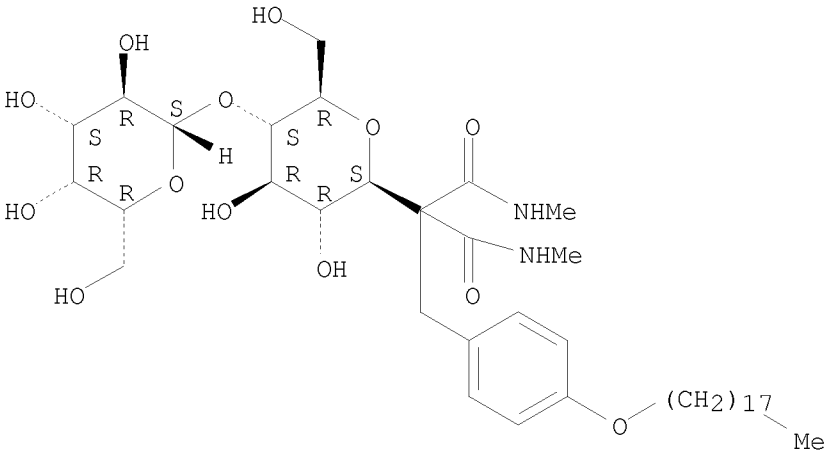
RN 660850-39-5 CAPLUS
CN Propanediamide, 2-β-D-galactopyranosyl-N,N'-dimethyl-2-[[4-(octadecyloxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 660850-40-8 CAPLUS
CN Propanediamide, 2-(4-O-β-D-galactopyranosyl-β-D-glucopyranosyl)-N,N'-dimethyl-2-[[4-(octadecyloxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

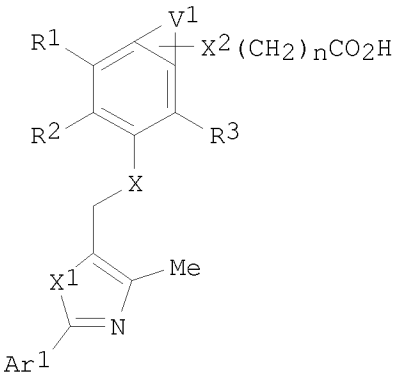
L6 ANSWER 2 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:719304 CAPLUS
DOCUMENT NUMBER: 139:246020
TITLE: Preparation of thiazolylmethoxyindoleacetates and related compounds as modulators of peroxisome proliferator activating receptor (PPAR) activity
INVENTOR(S): Cheng, Xue-min; Filzen, Gary Frederick; Geyer, Andrew George; Lee, Chitase; Trivedi, Bharat Kalidas
PATENT ASSIGNEE(S): Warner-Lambert Company Llc, USA
SOURCE: PCT Int. Appl., 131 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003074051	A1	20030912	WO 2003-IB882	20030303 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20030207915	A1	20031106	US 2002-324266	20021219 <--
US 6867224	B2	20050315		
CA 2478164	A1	20030912	CA 2003-2478164	20030303 <--
AU 2003207914	A1	20030916	AU 2003-207914	20030303 <--
EP 1480641	A1	20041201	EP 2003-704916	20030303
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003008202	A	20041221	BR 2003-8202	20030303
JP 2005527509	T	20050915	JP 2003-572568	20030303
MX 2004PA08627	A	20041206	MX 2004-PA8627	20040906

US 20050113422	A1	20050526	US 2004-20391		20041222
US 20050107442	A1	20050519	US 2004-25271		20041224
US 7109222	B2	20060919			
PRIORITY APPLN. INFO.:			US 2002-362411P	P	20020307
			US 2002-324266	A3	20021219
			WO 2003-IB882	W	20030303

OTHER SOURCE(S): MARPAT 139:246020

GI



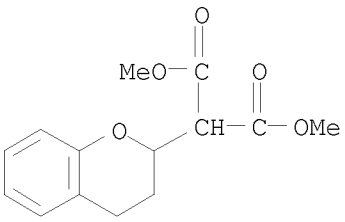
I

AB Title compds. [I; V1 = (unsatd.) (substituted) (heteroatom-containing) hydrocarbon chain having 3-6 atoms; X, X1 = O, S; X2 = absent, O, S, NR4; Ar1 = (substituted) aryl, heteroaryl; R1, R2, R3 = H, alkyl, alkoxy, thioalkoxy, O(CH2)pCF3, halo, NO2, cyano, OH, SH, CF3, S(O)pAlkyl, SOpAryl, (CH2)mOR4, (CH2)mNR5R6, COR4, CO2H, CO2R4, NR5R6; R1R2 form (substituted) (unsatd.) cycloalkyl, heterocycloalkyl; R4 = H, alkyl, alkenyl, alkynyl, aryl; R5, R6 = H, alkyl, alkenyl, alkynyl, cycloalkyl, SO2Alkyl, SO2Aryl; R5R6 form 4-7 membered ring having 0-3 heteroatoms; m = 0-5; n = 0-5; p = 0-2], were prepared Thus, 5-mercaptoindan-2-carboxylic acid Me ester (preparation given), 5-chloromethyl-4-methyl-2-(4-trifluoromethylphenyl)thiazole, and Cs2CO3 were stirred overnight in MeCN to give Me 5-[4-methyl-2-(4-trifluoromethylphenyl)thiazol-5-ylmethylsulfanyl]indan-2-carboxylate. The latter was refluxed overnight with LiOH.H2O in MeOH/THF to give 5-[4-methyl-2-(4-trifluoromethylphenyl)thiazol-5-ylmethylsulfanyl]indan-2-carboxylic acid. In a transient transfections assay using the HepG2 hepatoma cell line, the latter showed EC50 = 177.7 nM and 384 nM for Hep G2-hβ and Hep G2-hα, resp.

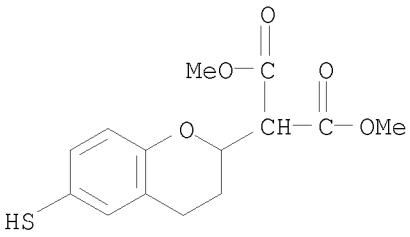
IT 600166-86-7P 600166-87-8P 600166-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazolylmethoxyindoleacetates and related compds. as modulators of peroxisome proliferator activating receptor (PPAR) activity)

RN 600166-86-7 CAPLUS

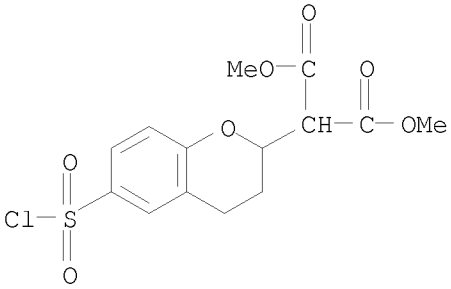
CN Propanedioic acid, (3,4-dihydro-2H-1-benzopyran-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 600166-87-8 CAPLUS
CN Propanedioic acid, (3,4-dihydro-6-mercapto-2H-1-benzopyran-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 600166-88-9 CAPLUS
CN Propanedioic acid, [6-(chlorosulfonyl)-3,4-dihydro-2H-1-benzopyran-2-yl]-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:366735 CAPLUS
DOCUMENT NUMBER: 137:140704
TITLE: An easy route to 2-amino-β-C-glycosides by conjugate addition to 2-nitroglycals
AUTHOR(S): Pachamuthu, Kandasamy; Gupta, Anuradha; Das, Jagattaran; Schmidt, Richard R.; Vankar, Yashwant D.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kanpur, 208 016, India
SOURCE: European Journal of Organic Chemistry (2002), (9), 1479-1483
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:140704

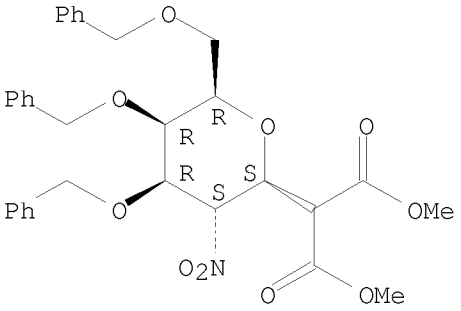
AB 2-Nitroglycals were found to undergo conjugate addition with a variety of stabilized soft carbanions. The Michael adducts from galactal derivs. were converted into bicyclic lactams.

IT 444666-44-8P 444666-51-7P 444666-54-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-amino-β-C-glycosides and bicyclic lactams via Michael addition of carbanions to 2-nitroglycals as a key step)

RN 444666-44-8 CAPLUS

CN Propanedioic acid, [2-deoxy-2-nitro-3,4,6-tris-O-(phenylmethyl)-β-D-galactopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

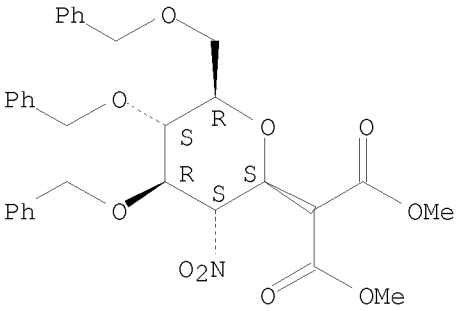
Absolute stereochemistry. Rotation (+).



RN 444666-51-7 CAPLUS

CN Propanedioic acid, [2-deoxy-2-nitro-3,4,6-tris-O-(phenylmethyl)-β-D-glucopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

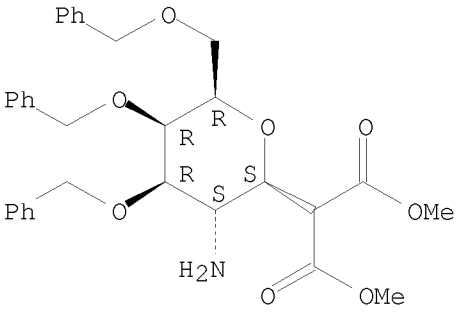
Absolute stereochemistry. Rotation (-).



RN 444666-54-0 CAPLUS

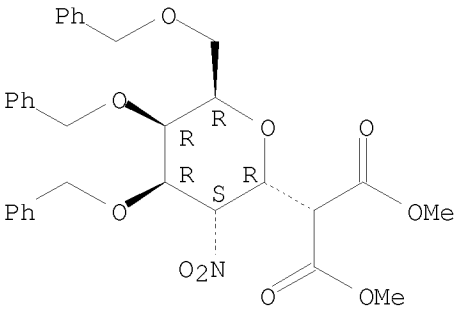
CN Propanedioic acid, [2-amino-2-deoxy-3,4,6-tris-O-(phenylmethyl)-β-D-galactopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



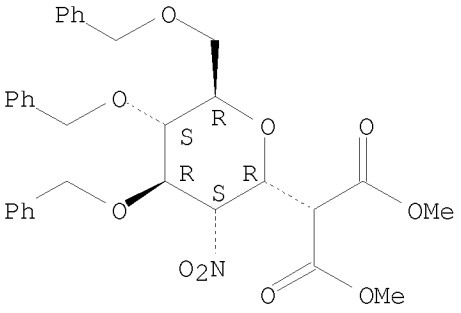
IT 444666-45-9P 444666-52-8P 444666-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-amino-β-C-glycosides and bicyclic lactams via Michael addition of carbanions to 2-nitroglycals as a key step)
RN 444666-45-9 CAPLUS
CN Propanedioic acid, [2-deoxy-2-nitro-3,4,6-tris-O-(phenylmethyl)-α-D-galactopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



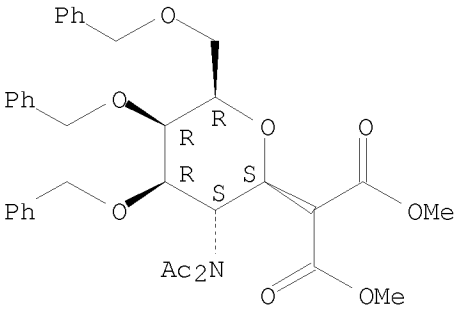
RN 444666-52-8 CAPLUS
CN Propanedioic acid, [2-deoxy-2-nitro-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 444666-60-8 CAPLUS
CN Propanedioic acid, [2-deoxy-2-(diacetylamino)-3,4,6-tris-O-(phenylmethyl)-β-D-galactopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

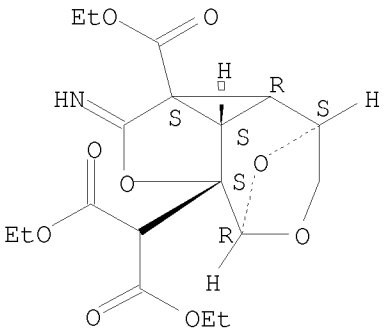
L6 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:916992 CAPLUS
DOCUMENT NUMBER: 136:247799
TITLE: Reaction of iodolevoglucosenone with ethyl cyanoacetate under Michael reaction conditions
AUTHOR(S): Gorobets, E. V.; Spirikhin, L. V.; Tzypysheva, I. P.; Miftakhov, M. S.; Valeev, F. A.
CORPORATE SOURCE: Institute of Organic Chemistry, Ufa Scientific Center, Russian Academy of Sciences, Ufa, 450054, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2001), 37(8), 1088-1092
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:247799

AB The reaction of iodolevoglucosenone with the anion of Et cyanoacetate via succession of tandem intramol. reactions leads to formation of tricyclic cyclopropanolevoglucosenone or tetracyclic imine.

IT 227776-94-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael reaction of iodolevoglucosenone with Et cyanoacetate in preparation of tricyclic cyclopropanolevoglucosenone or tetracyclic imine)

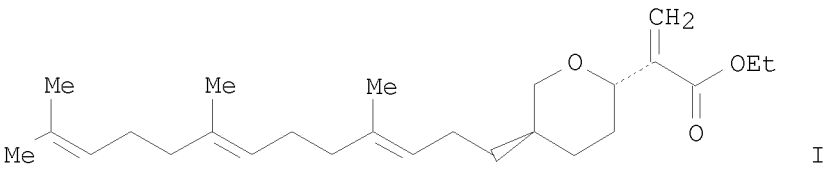
RN 227776-94-5 CAPLUS
CN Propanedioic acid, [(2aS,2bR,3S,6R,6aS,6bS)-2a-(ethoxycarbonyl)hexahydro-2-imino-3,6-epoxy-1,5-dioxacycloprop[cd]azulen-6a(6H)-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:781672 CAPLUS
DOCUMENT NUMBER: 136:102261
TITLE: Stereoselective formation of trans-2,5-disubstituted tetrahydropyrans by intramolecular nucleophilic substitution and a computational study at the AM1 level
AUTHOR(S): Takagi, Ryukichi; Nishitani, Hiroko; Takenami, Sigeharu; Okada, Kazumasa; Kojima, Satoshi; Ohkata, Katsuo
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2001), 74(10), 1901-1907
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:102261
GI



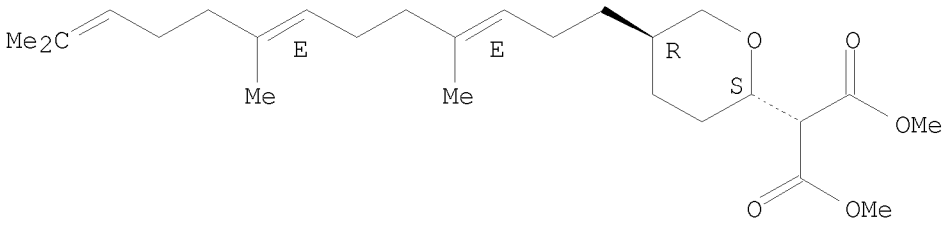
I

AB The synthesis of 2,5-disubstituted tetrahydropyrans, e.g. I, bearing a hydrophobic moiety at the C5 position from (E)- and (Z)-7-hydroxy-6-substituted 2,3-unsatd. esters by way of intramol. nucleophilic substitution proceeded with high stereoselectivity. A theor. study at the AM1 level of the cyclization reaction suggested that the reaction is kinetically controlled and that the preferred path for the cyclization reaction proceeds via a transition state in which 1,3-diaxial-like repulsions are minimized to give the trans product in accordance with exptl. results.

IT 389632-54-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective formation of trans-2,5-disubstituted tetrahydropyrans by intramol. nucleophilic substitution and a computational study at the AM1 level)

RN 389632-54-6 CAPLUS
CN Propanedioic acid, [(2R,5S)-tetrahydro-5-[(3E,7E)-4,8,12-trimethyl-3,7,11-tridecatrienyl]-2H-pyran-2-yl]-, dimethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

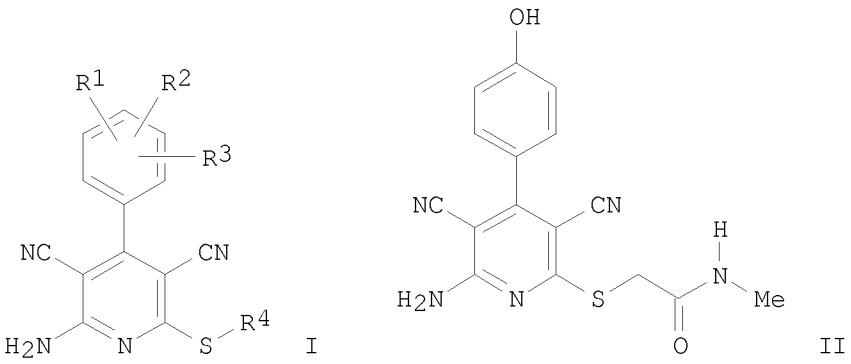
L6 ANSWER 6 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:265394 CAPLUS
DOCUMENT NUMBER: 134:295744
TITLE: Substituted 2-thio-3,5-dicyano-4-aryl-6-aminopyridines and the use thereof as adenosine receptor ligands
INVENTOR(S): Rosentreter, Ulrich; Henning, Rolf; Bauser, Marcus; Kraemer, Thomas; Vaupel, Andrea; Huebsch, Walter; Dembowsky, Klaus; Salcher-Schraufstaetter, Olga; Stasch, Johannes-Peter; Krahn, Thomas; Perzborn, Elisabeth
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: PCT Int. Appl., 316 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001025210	A2	20010412	WO 2000-EP9153	20000919 <--
WO 2001025210	A3	20011011		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19947154	A1	20011004	DE 1999-19947154	19991001 <--
CA 2386147	A1	20010412	CA 2000-2386147	20000919 <--
BR 2000014679	A	20020702	BR 2000-14679	20000919 <--
EP 1240145	A2	20020918	EP 2000-967705	20000919 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
HU 2002002810	A2	20021228	HU 2002-2810	20000919 <--
HU 2002002810	A3	20030228		
JP 2003511371	T	20030325	JP 2001-528156	20000919 <--
EE 200200175	A	20030415	EE 2002-175	20000919 <--
AU 775159	B2	20040722	AU 2000-77780	20000919
RU 2267482	C2	20060110	RU 2002-111569	20000919
ZA 2002001806	A	20030305	ZA 2002-1806	20020305 <--
IN 2002MN00331	A	20050318	IN 2002-MN331	20020319
NO 2002001449	A	20020507	NO 2002-1449	20020322 <--
NO 323848	B1	20070709		

BG 106546	A	20030331	BG 2002-106546		20020322 <--
MX 2002PA03271	A	20021104	MX 2002-PA3271		20020327 <--
US 7135486	B1	20061114	US 2002-110284		20020819
US 20060264432	A1	20061123	US 2006-359927		20060221
IN 2007MN01333	A	20071026	IN 2007-MN1333		20070903
KR 2007106051	A	20071031	KR 2007-723773		20071017
PRIORITY APPLN. INFO.:			DE 1999-19947154	A	19991001
			WO 2000-EP9153	W	20000919
			IN 2002-MN331	A3	20020319
			KR 2002-704179	A3	20020330
			US 2002-110284	A3	20020819

OTHER SOURCE(S): MARPAT 134:295744

GI



AB The invention relates to compds. I, a method for their production, and their use as pharmacol. effective substances for a broad spectrum of medical indications [wherein: R1, R2, R3 = H, OH, (un)substituted alkyl, aryl, alkoxy, O(CH2)0-2CH:CH2, halo, NO2, cyano, COR5, CONR6R7, NR6R7, etc.; R4 = (un)substituted alkyl or alkenyl, or 5- to 7-membered (un)saturated NOS heterocyclyl; R5 = H, OH, (un)substituted alkyl, cycloalkyl, alkoxy, aryl, aryloxy, aralkoxy, 5- to 7-membered (un)saturated heterocyclyl, or 5- to 6-membered NOS heteroaryl; R6, R7 = H, (un)substituted alkyl, aryl, or 5- to 6-membered NOS heteroaryl; or NR6R7 = 5- to 7-membered (un)saturated NOS heterocyclyl; including tautomers, salts, hydrates, and alcoholates; with many specific exclusions]. In particular, selective adenosine receptor ligands are provided, preferably selective adenosine A1, adenosine A2a, and/or adenosine A2b receptor ligands. The compds. are useful for the prophylaxis and/or the treatment of diseases, especially cardiovascular diseases, diseases of the urogenital region, diseases of the respiratory tract, inflammatory and neuroinflammatory diseases, diabetes, especially pancreatic diabetes, neurodegenerative diseases, pain states, and cancer, as well as liver fibrosis and cirrhosis. Over 400 compds. were synthesized on a preparative scale, and 375 addnl. compds. were prepared on a 10-μmol scale. For instance, title compound II was prepared in 66.3% yield by thioetherification of the corresponding pyridinethiol with MeNHCOCH2Br using NaHCO3 in DMF at room temperature II had a marked agonist activity on cells expressing human adenosine A2b receptors, and nearly no activity against cells expressing A2a receptors. Compds. I also selectively reduced coronary perfusion pressure in narcotized rats at concns. of 10-7 to 10-6 g/mL.

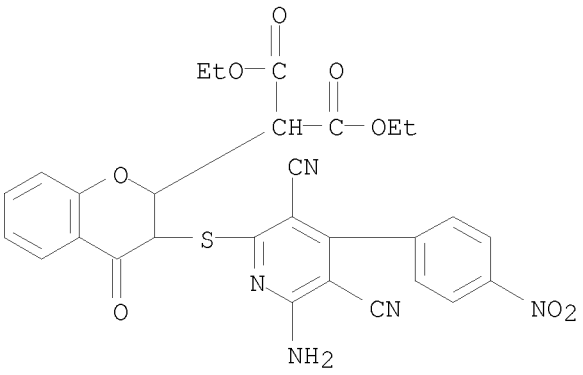
IT 333965-30-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of substituted thiodicyanoarylaminopyridines as adenosine receptor agonists)

RN 333965-30-3 CAPLUS

CN Propanedioic acid, [3-[[6-amino-3,5-dicyano-4-(4-nitrophenyl)-2-pyridinyl]thio]-3,4-dihydro-4-oxo-2H-1-benzopyran-2-yl]-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:812644 CAPLUS

DOCUMENT NUMBER: 134:71816

TITLE: Transformations in carbohydrate chemistry 1. Synthesis of C-2 methylene O- and C-glycosides and sugar derived α-methylene-δ-valerolactones from C-2-acetoxymethyl glycals

AUTHOR(S): Gupta, Anuradha; Vankar, Yashwant D.

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kanpur, 208 016, India

SOURCE: Tetrahedron (2000), 56(43), 8525-8531
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:71816

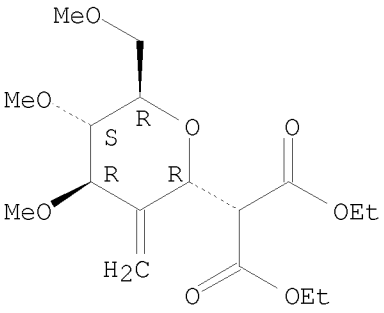
AB C-2-Methylene O- and C-glycosides are readily synthesized from C-2-acetoxymethyl glycals using Nafion-H, montmorillonite K-10, LiClO4 (0.07 M) in dichloromethane and Pd(PPh3)4 as catalysts. Exclusive α or β selectivities have been observed with various primary, secondary and tertiary alcs., phenols and di-Et malonate. Further, C-2-acetoxymethyl glycals are also converted into corresponding α-methylene-δ-valerolactones in good yields in one step using m-CPBA in the presence of BF3·Et2O.

IT 314249-26-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of C-2 methylene O- and C-glycosides and α-methylene-δ-valerolactones from C-2-acetoxymethyl glycals)

RN 314249-26-8 CAPLUS

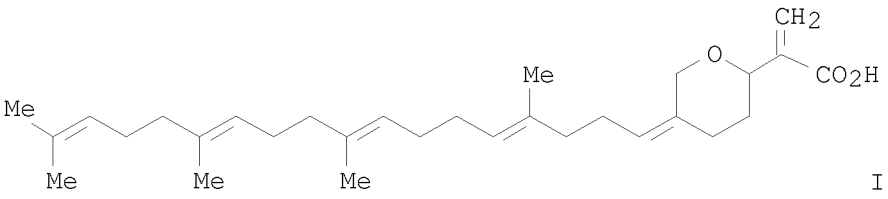
CN Propanedioic acid, (2-deoxy-3,4,6-tri-O-methyl-2-methylene-α-D-arabino-hexopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:497824 CAPLUS
DOCUMENT NUMBER: 131:337198
TITLE: Triterpenoid total synthesis. Part 4. Synthesis of (±)-hippospongic acid A, a triterpene isolated from the marine sponge Hippospongia sp.
AUTHOR(S): Takikawa, Hirosato; Koizumi, Junko; Kato, Yuko; Mori, Kenji
CORPORATE SOURCE: Shinjuku-ku, Kagurazaka 1-3, Department of Chemistry, Science University of Tokyo, Tokyo, 162-8601, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2271-2275
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:337198
GI



I

AB Hippospongic acid A (I), a triterpene metabolite of a marine sponge Hippospongia sp. with inhibitory activity against gastrulation of starfish embryos, was synthesized as its racemate by starting from (2E,6E)-farnesol, (E,E)-Me(CMe:CHCH2CH2)2CMe:CHCH2OH.

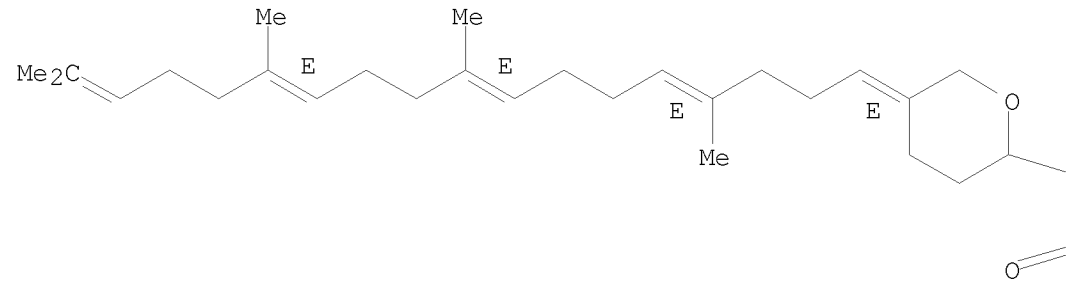
IT 249927-30-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of hippospongic acid A as its racemate by starting from (E,E)-farnesol)

RN 249927-30-8 CAPLUS

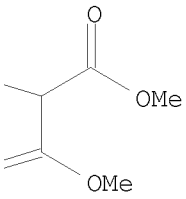
CN Propanedioic acid, [(5E)-tetrahydro-5-[(4E,8E,12E)-4,9,13,17-tetramethyl-4,8,12,16-octadecatetraenylidene]-2H-pyran-2-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

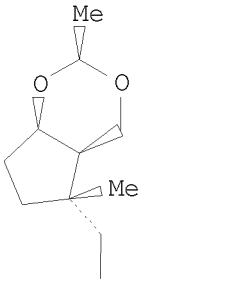


PAGE 1-B



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:482771 CAPLUS
DOCUMENT NUMBER: 131:286661
TITLE: Radical-Mediated Diastereoselective Construction of a Chiral Synthon for Synthesis of Dolabellanes
AUTHOR(S): Zhu, Qiang; Fan, Kai-Yi; Ma, Hong-Wei; Qiao, Li-Xin; Wu, Yu-Lin; Wu, Yikang
CORPORATE SOURCE: State Key Laboratory of Bio-organic Natural Products Chemistry, Shanghai Institute of Organic Chemistry Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Organic Letters (1999), 1(5), 757-759
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:286661
GI



I

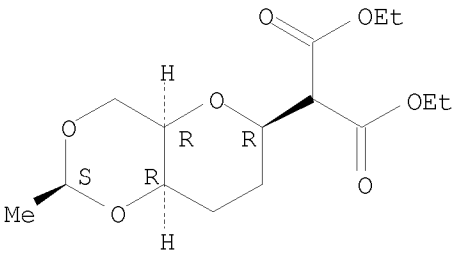
AB A useful trans-substituted multifunctional cyclopentane (I) with a chiral quaternary center was selectively synthesized by free radical Michael addition to the (Z)-propionate or -malonate derivs. The stereoselectivity could be reversed by changing the configuration of the double bond.

IT 246853-37-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(radical-mediated diastereoselective construction of a chiral synthon for synthesis of dolabellanes)

RN 246853-37-2 CAPLUS

CN D-xylo-Octonic acid, 3,7-anhydro-2,4,5-trideoxy-2-(ethoxycarbonyl)-6,8-O-(1S)-ethylidene-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:347540 CAPLUS

DOCUMENT NUMBER: 131:59072

TITLE: Reactions of 3-iodolevoglucosenone with sodium derivatives of some CH acids. Chiral cyclopropanes and stable oxetenes

AUTHOR(S): Valeev, F. A.; Gorobets, E. V.; Miftakhov, M. S.

CORPORATE SOURCE: Institute of Organic Chemistry, Ufa Research Center of the Russian Academy of Sciences, Ufa, 450054, Russia

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1999), 48(1), 152-156
CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:59072

AB 3-Iodolevoglucosenone reacts with the sodium derivative of Et cyanoacetate at -60°C to give a tetra-substituted cyclopropane derivative; similar

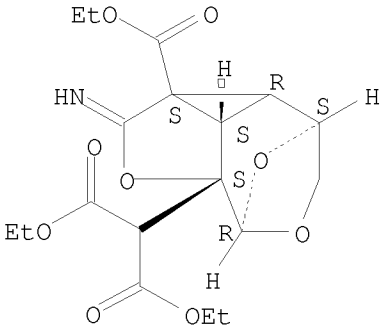
reactions of the sodium derivs. of Et acetoacetate and acetylacetone at -60°C afford the expected transformed Michael adducts, while at 20°C, O,C-dialkylated products of the oxetene series are formed.

IT 227776-94-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael addition of iodolevoglucosenone with sodium derivs. of some CH acids in preparation of chiral cyclopropane and stable oxetene sugars)

RN 227776-94-5 CAPLUS

CN Propanedioic acid, [(2aS,2bR,3S,6R,6aS,6bS)-2a-(ethoxycarbonyl)hexahydro-2-imino-3,6-epoxy-1,5-dioxacycloprop[cd]azulen-6a(6H)-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:257568 CAPLUS

DOCUMENT NUMBER: 128:321842

TITLE: Synthesis of benzylated (R)- and (S)-aminoethyl-C-α-D-mannosides as conformationally restricted building blocks for the preparation of E- and P-selectin antagonists

AUTHOR(S): Roche, Didier; Banteli, Rolf; Winkler, Tammo; Casset, Florence; Ernst, Beat

CORPORATE SOURCE: Novartis Pharma Corp., East Hanover, NJ, 07936, USA

SOURCE: Tetrahedron Letters (1998), 39(17), 2545-2548
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

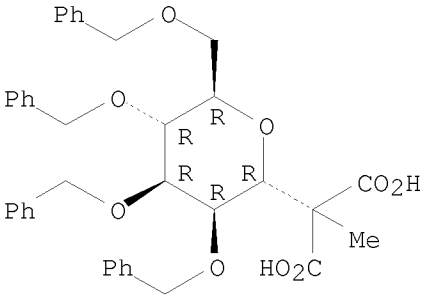
AB A straightforward synthesis for (R)- and (S)-aminoethyl-C-α-D-mannosides has been developed. The conformationally restricted mannosides serve as building blocks for the synthesis of a new class of selectin antagonists of type A.

IT 207107-96-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzylated (R)- and (S)-aminoethyl-C-mannosides as conformationally restricted building blocks for the preparation of E- and P-selectin antagonists)

RN 207107-96-8 CAPLUS

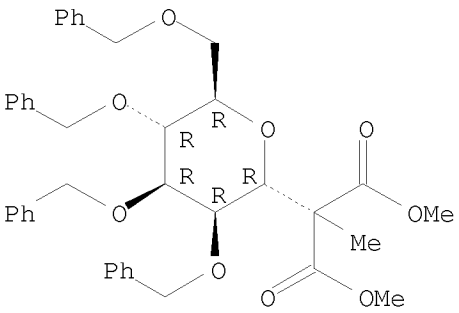
CN Propanedioic acid, methyl[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 207107-95-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzylated (R)- and (S)-aminoethyl-C-mannosides as conformationally restricted building blocks for the preparation of E- and P-selectin antagonists)
RN 207107-95-7 CAPLUS
CN Propanedioic acid, methyl[2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-mannopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

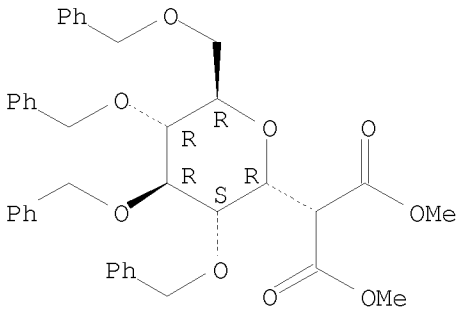
L6 ANSWER 12 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:603810 CAPLUS
DOCUMENT NUMBER: 127:248294
TITLE: Anionic Additions to Glycosyl Iodides: Highly Stereoselective Syntheses of β C-, N-, and O-Glycosides
AUTHOR(S): Gervay, Jacquelyn; Hadd, Michael J.
CORPORATE SOURCE: Department of Chemistry, University of Arizona, Tucson, AZ, 85721, USA
SOURCE: Journal of Organic Chemistry (1997), 62(20), 6961-6967
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:248294
AB Classically, glycosyl halides are activated as glycosyl donors by metal chelation under Koenigs-Knorr or Helferich conditions. These reactions often proceed through oxonium formation, and the stereochem. outcome is

dictated by the anomeric effect and/or the nature of the protecting group on the C2 hydroxyl. Alternatively, glycosyl halides may undergo direct displacement of the halide by an incoming nucleophile in an SN2 mechanism. The latter reaction is far less common, and before this study it was primarily performed with glycosyl bromides. Having recently shown that both α and β glycosyl iodides could be efficiently generated, we embarked upon an investigation of nucleophilic addns. to glycosyl iodides. The studies reported herein show that addns. of stabilized anions to α-glycosyl iodides proceed with inversion of stereochem. to give β-glycosides, even in the absence of a C2 participatory group. Glucosyl, galactosyl, and mannosyl iodides were studied, and the combined results indicate that the reactivity of 2,3,4,6-tetra-O-benzyl-α-D-galactosyl iodide > 2,3,4,6-tetra-O-benzyl-α-D-glucosyl iodide > 2,3,4,6-tetra-O-benzyl-α-D-mannosyl iodide. Both the glucosyl and galactosyl iodides are susceptible to E-2 elimination when treated with highly basic anions. In contrast, the mannosyl iodide undergoes substitution to give the 1,2 cis configuration. The overall sequence involves reaction of an anomeric acetate with trimethylsilyl iodide with in vacuo removal of the resulting trimethylsilyl acetate. The iodide is then treated with a nucleophile without further characterization. A variety of nucleophiles were stereoselectively added to the glycosyl halides providing β-, C-, N-, and O-glycosides.

IT 96689-83-7P 195874-76-1P 195874-77-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(anionic addns. to glycosyl iodides in highly stereoselective syntheses of glycosides)

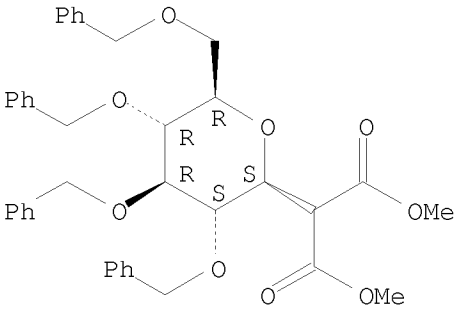
RN 96689-83-7 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



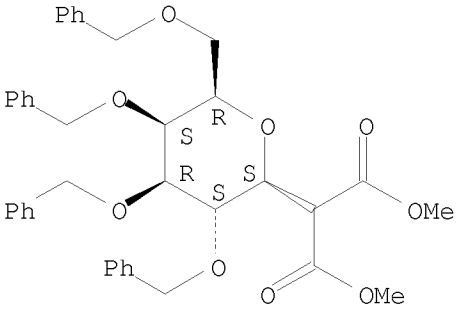
RN 195874-76-1 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-β-D-glucopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



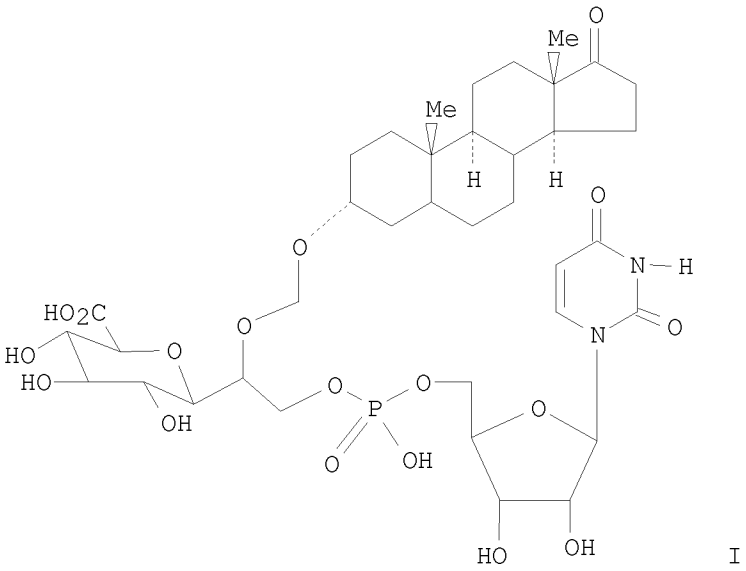
RN 195874-77-2 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-β-D-galactopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:423743 CAPLUS
DOCUMENT NUMBER: 127:121959
TITLE: Synthesis and inhibitory effect of a trisubstrate transition state analog for UDP glucuronosyltransferases
AUTHOR(S): Timmers, C. M.; Dekker, M.; Buijsman, R. C.; Van Der Marel, G. A.; Ethell, B.; Anderson, G.; Burchell, B.; Mulder, G. J.; Van Boom, J. H.
CORPORATE SOURCE: Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, Leiden, 2300 RA, Neth.
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(12), 1501-1506
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

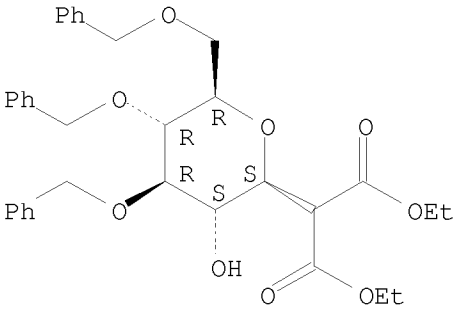
AB Tri-substrate UGT (UDP glucuronosyltransferase) transition state analog glucuronate uridine phosphate I is readily accessible by nucleophilic ring-opening of 1,2-anhydroglucose precursor with diethylmalonate anion followed by reduction of the Et ester moieties. I diastereomers show a different inhibition pattern for several UGT isoforms, indicating isoenzyme selectivity. Moreover, C7τ-epimers I exert a different inhibitory effect on UGT2B15.

IT 192753-12-1P 192753-13-2P 192753-14-3P
192753-15-4P 192753-16-5P 192753-17-6P
192753-18-7P 192753-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and inhibitory effect of a trisubstrate transition state analog for UDP glucuronosyltransferases)

RN 192753-12-1 CAPLUS

CN Propanedioic acid, [3,4,6-tris-O-(phenylmethyl)-β-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

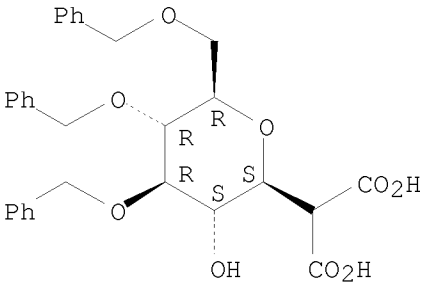
Absolute stereochemistry.



RN 192753-13-2 CAPLUS

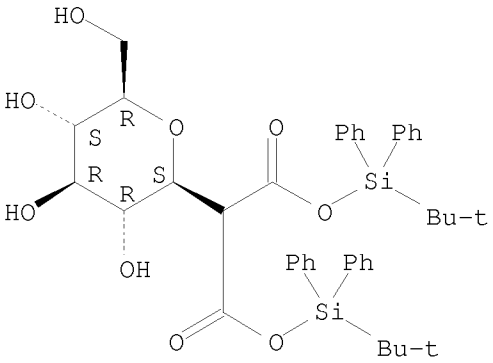
CN Propanedioic acid, [3,4,6-tris-O-(phenylmethyl)-β-D-glucopyranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



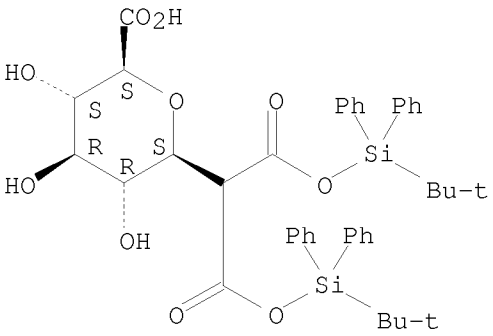
RN 192753-14-3 CAPLUS
CN Propanedioic acid, β-D-glucopyranosyl-, bis[(1,1-dimethylethyl)diphenylsilyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



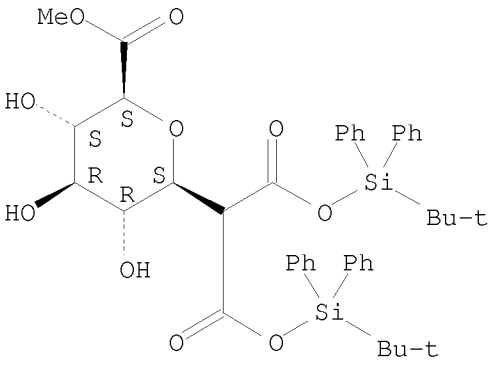
RN 192753-15-4 CAPLUS
CN D-glycero-D-gulo-Octaric acid, 3,7-anhydro-2-deoxy-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]carbonyl]-, 1-[(1,1-dimethylethyl)diphenylsilyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



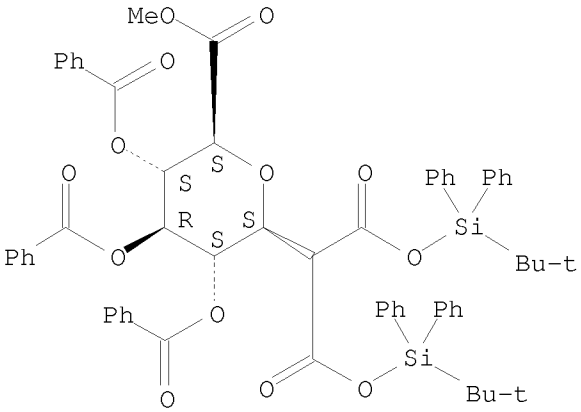
RN 192753-16-5 CAPLUS
CN D-glycero-D-gulo-Octaric acid, 3,7-anhydro-2-deoxy-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]carbonyl]-, 1-[(1,1-dimethylethyl)diphenylsilyl] 8-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



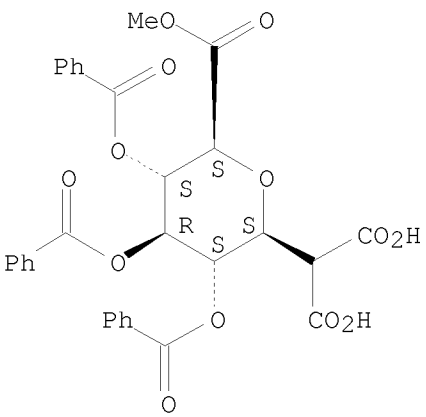
RN 192753-17-6 CAPLUS
CN D-glycero-D-gulo-Octaric acid, 3,7-anhydro-2-deoxy-2-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]carbonyl]-, 1-[(1,1-dimethylethyl)diphenylsilyl] 8-methyl ester, tribenzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



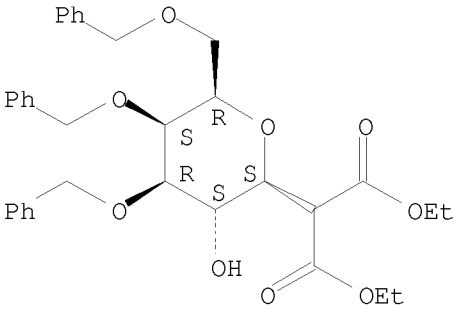
RN 192753-18-7 CAPLUS
CN D-glycero-D-gulo-Octaric acid, 3,7-anhydro-2-carboxy-2-deoxy-, 8-methyl ester, tribenzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



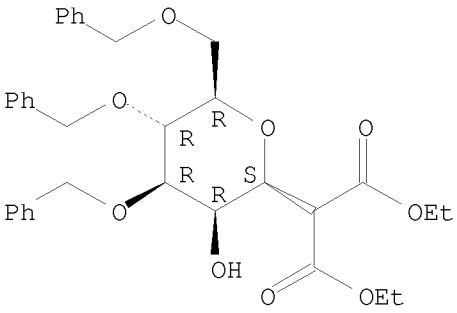
RN 192753-22-3 CAPLUS
CN Propanedioic acid, [3,4,6-tris-O-(phenylmethyl)-β-D-galactopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



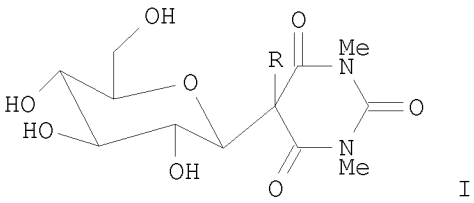
IT 192753-23-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and inhibitory effect of a trisubstrate transition state analog for UDP glucuronosyltransferases)
RN 192753-23-4 CAPLUS
CN Propanedioic acid, [3,4,6-tris-O-(phenylmethyl)-β-D-mannopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:13473 CAPLUS
DOCUMENT NUMBER: 122:56357
TITLE: On the synthesis of C-glycosyl compounds containing double bonds without the use of protecting groups
AUTHOR(S): Wulff, Guenter; Clarkson, Guy
CORPORATE SOURCE: Inst. Org. Chem. Makromol. Chem., Heinrich-Heine Univ., Duesseldorf, 40225, Germany
SOURCE: Carbohydrate Research (1994), 257(1), 81-95
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:56357
GI



I

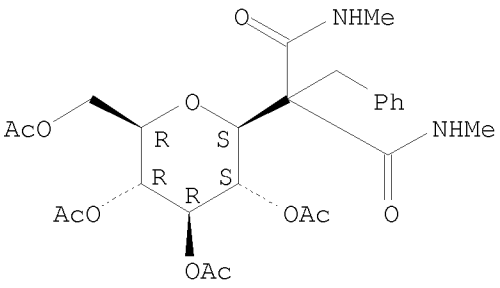
AB A new range of C-glycosyl compds. carrying double bonds have been synthesized as potential monomers for the preparation of polyvinyl-saccharides. The syntheses were performed without the use of protecting groups and mostly in water as solvent. The starting material was the easily accessible 5-β-D-glycopyranosyl-1,3-dimethylbarbituric acid sodium salt I (R = Na) (obtained from D-glucose and 1,3-dimethylbarbituric acid in water). The alkylation reaction of I (R = Na) at C-5 of the barbiturate moiety was studied in detail. It works well with benzylic bromides in Me2SO and with allylic or benzylic bromides by an ultrasound/phase transfer catalyst-promoted alkylation in water. The resulting 5,5-dialkylated barbiturates, e.g. I (R = CH2C6H4-R1, R1 = H, CH:CH2, CH2CH2Br; R = CH2CR2:CH2, R2 = H, Ph, CO2Me), undergo an unusually facile and specific cleavage of the barbituric ring, losing the c-2 carbonyl, to yield novel mols. with a diamide moiety.

IT 160055-68-5P 160055-69-6P 160055-70-9P 160055-71-0P 160055-72-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 160055-68-5 CAPLUS

CN Propanediamide, N,N'-dimethyl-2-(phenylmethyl)-2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

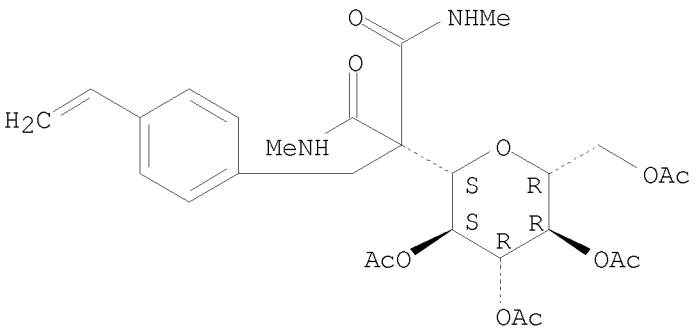
Absolute stereochemistry.



RN 160055-69-6 CAPLUS

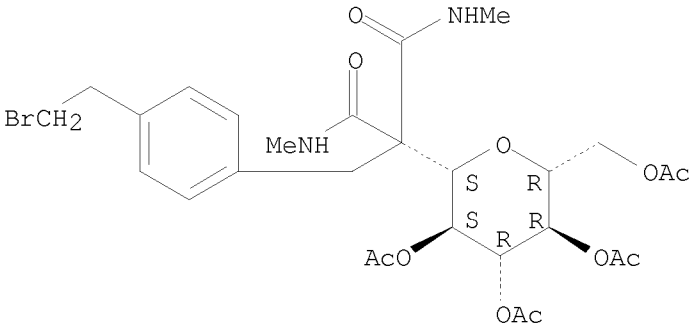
CN Propanediamide, 2-[(4-ethenylphenyl)methyl]-N,N'-dimethyl-2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



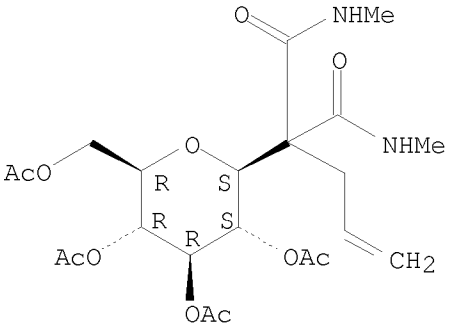
RN 160055-70-9 CAPLUS
CN Propanediamide, 5-[[4-(2-bromoethyl)phenyl]methyl]-N,N'-dimethyl-2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



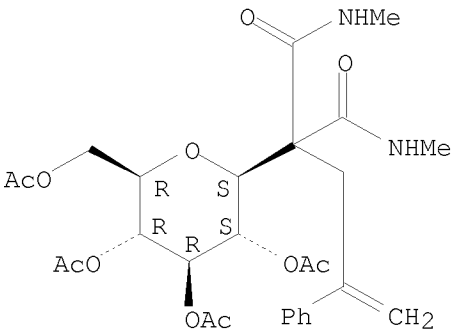
RN 160055-71-0 CAPLUS
CN Propanediamide, N,N'-dimethyl-2-(2-propenyl)-2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

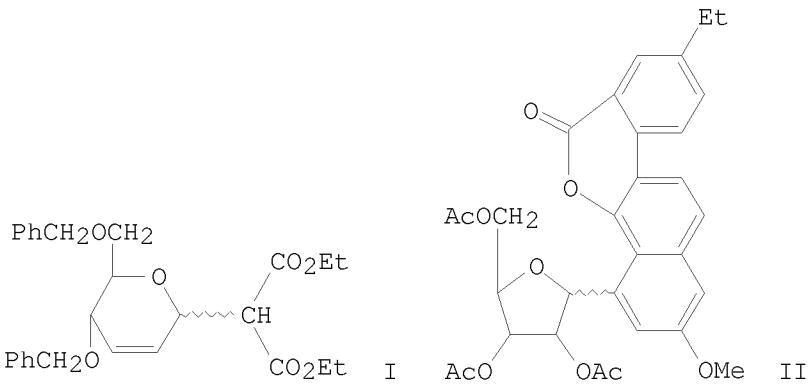


RN 160055-72-1 CAPLUS
CN Propanediamide, N,N'-dimethyl-2-(2-phenyl-2-propenyl)-2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

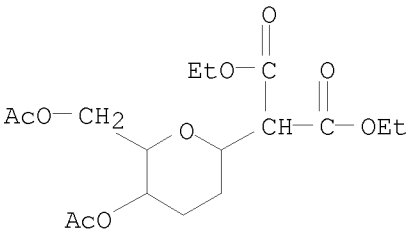


L6 ANSWER 15 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:449758 CAPLUS
DOCUMENT NUMBER: 119:49758
TITLE: Assignment of anomeric configuration of C-glycopyranosides and C-glycofuranosides. A proton, carbon-13, and nuclear Overhauser enhancement spectrometric study
AUTHOR(S): Brakta, Mohamed; Farr, Roger N.; Chaguir, Brahim; Massiot, Georges; Lavaud, Catherine; Anderson, William R., Jr.; Sinou, Denis; Daves, G. Doyle, Jr.
CORPORATE SOURCE: ESCIL, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
SOURCE: Journal of Organic Chemistry (1993), 58(11), 2992-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

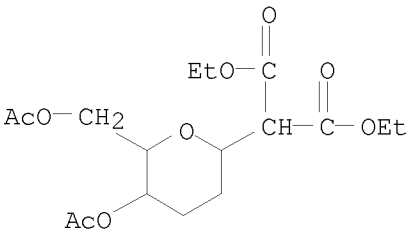


AB The utility of 1H, 13C, and NOE spectrometries for assignment on C-glycopyranosides, e.g. I, and C-glycofuranosides, e.g. II, to α- or β-anomer series has been assessed. While all of these data have been used for assignment of anomeric configuration of C-glycosides, this study demonstrates that the NOE obtained by irradiation of H1' is uniquely reliable. For β-C-glycosides, in which H1' and H5' (C-glycopyranosides) or H1' and H4' (C-glycofuranosides) are on the same face of the carbohydrate ring, irradiation of H1' gives rise to the appropriate NOE. In no instance dose irradiation of an α C-glycoside give rise to such an effect.

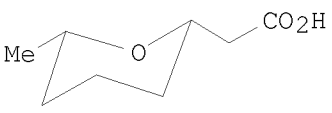
IT 141407-03-6P 141407-04-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anomeric configuration of)
RN 141407-03-6 CAPLUS
CN Propanedioic acid, (4,6-di-O-acetyl-2,3-dideoxy-α-D-erythro-hexopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 141407-04-7 CAPLUS
CN Propanedioic acid, (4,6-di-O-acetyl-2,3-dideoxy-β-D-erythro-hexopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 16 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:634351 CAPLUS
DOCUMENT NUMBER: 117:234351
ORIGINAL REFERENCE NO.: 117:40551a,40554a
TITLE: Palladium catalyzed tandem allylic substitution methodology in the synthesis of a component of civet
AUTHOR(S): Bredenkamp, Martin W.; Holzapfel, Cedric W.; Toerien, Francois
CORPORATE SOURCE: Dep. Chem. Biochem., Rand Afrikaans Univ., Johannesburg, S. Afr.
SOURCE: Synthetic Communications (1992), 22(17), 2447-57
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:234351
GI



I

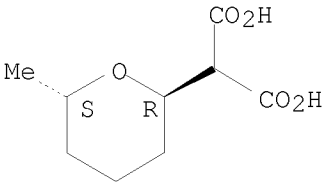
AB A facile synthesis of a component of civet I is reported in which the key step involves palladium catalyzed introduction of the acetic acid substituent in the C-1 position of a pseudo-rhamnal derivative

IT 144491-64-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 144491-64-5 CAPLUS

CN Propanedioic acid, (tetrahydro-6-methyl-2H-pyran-2-yl)-, (2R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 17 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:571747 CAPLUS

DOCUMENT NUMBER: 117:171747

ORIGINAL REFERENCE NO.: 117:29709a,29712a

TITLE: Synthesis of (2RS,4'R,8'R)-α-tocopherol and related compounds via a 2-chlorochroman.

AUTHOR(S): Cohen, Noal; Schaer, Beatrice; Scalone, Michelangelo

CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche, Inc., Nutley, NJ, 07110, USA

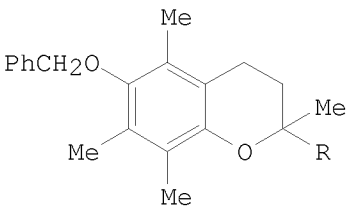
SOURCE: Journal of Organic Chemistry (1992), 57(21), 5783-5
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

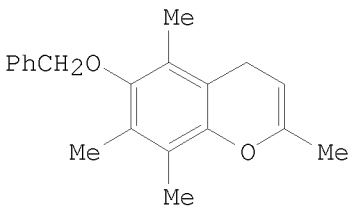
LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:171747

GI



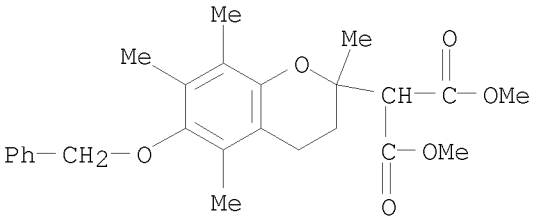
I



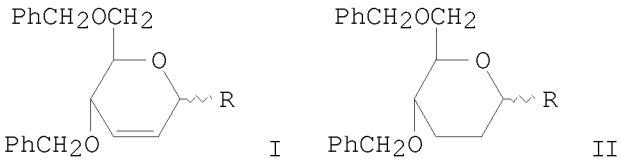
II

AB Coupling reactions of the novel 2-chlorochroman I (R = Cl) with various nucleophiles were examined in an effort to develop new pathways to antioxidant chromans of the tocopherol class. The reactivity pattern observed with this highly reactive electrophile involved in all cases, competitive elimination generating the chromene II as a major byproduct. Nonetheless, useful yields of coupling products I [R = (4R,8R)-4,8,12-trimethyldecyl, Et, CH2CH:CH2] were isolated when I (R = Cl) was treated with the corresponding Grignard reagents, in ether solution The benzyl ether I [R = (4R,8R)-4,8,12-trimethyldecyl] is a precursor to (2RS,4'R,8'R)-α-tocopherol.

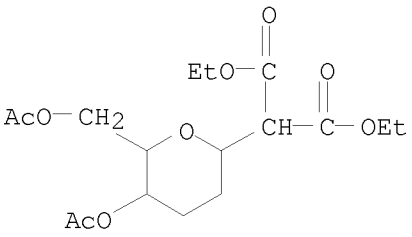
IT 114341-60-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from chloro(benzyloxy)tetramethylchroman)
RN 114341-60-5 CAPLUS
CN Propanedioic acid, [3,4-dihydro-2,5,7,8-tetramethyl-6-(phenylmethoxy)-2H-1-benzopyran-2-yl]-, dimethyl ester (9CI) (CA INDEX NAME)



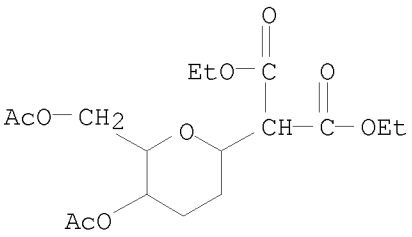
L6 ANSWER 18 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:255901 CAPLUS
DOCUMENT NUMBER: 116:255901
ORIGINAL REFERENCE NO.: 116:43407a,43410a
TITLE: Differentiation of anomeric C-glycosides by mass spectrometry using fast atom bombardment, mass-analyzed ion kinetic energy and collision-activated dissociation
AUTHOR(S): Brakta, Mohamed; Chaguir, Brahim; Sinou, Denis; Banoub, Joseph; Becchi, Michel
CORPORATE SOURCE: ESCIL, Univ. Claude Bernard Lyon, Villeurbanne, 69622, Fr.
SOURCE: Organic Mass Spectrometry (1992), 27(3), 331-9
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



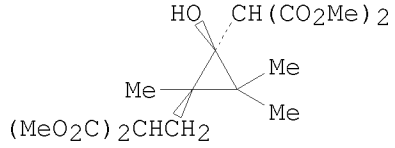
AB Pos.-ion fast atom bombardment mass spectrometry appears to be a useful method for the differentiation of anomeric C-glycosides, e.g. I [R = C(NO2)(CO2Et)2, CH(NO2)CO2Et] and II. The mass-analyzed ion kinetic energy (MIKE) and collision-activated dissociation (CAD) MIKE spectra of selected pos. ions can be used as fingerprints of the α- and β-anomers. The main fragmentation routes and particularly the formation of the [M - H]+ ion and the [M + M - PhCH2OH]+ ion were traced for each anomer.
IT 141407-03-6 141407-04-7
RL: PRP (Properties)
(fast-atom-bombardment mass spectra of)
RN 141407-03-6 CAPLUS
CN Propanedioic acid, (4,6-di-O-acetyl-2,3-dideoxy-α-D-erythro-hexopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



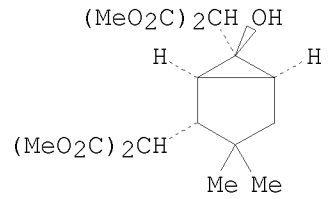
RN 141407-04-7 CAPLUS
CN Propanedioic acid, (4,6-di-O-acetyl-2,3-dideoxy-β-D-erythro-hexopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 19 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:20706 CAPLUS
DOCUMENT NUMBER: 116:20706
ORIGINAL REFERENCE NO.: 116:3647a,3650a
TITLE: Functional group hybrids. Reactivity of α'-nucleofuge α,β-unsaturated ketones. 2. Reactions with malonate anion. Concerning the mechanism of the Favorskii rearrangement
AUTHOR(S): Barbee, Thomas R.; Guy, Hedeel; Heeg, Mary Jane; Albizati, Kim F.
CORPORATE SOURCE: Dep. Chem., Wayne State Univ., Detroit, MI, 48202, USA
SOURCE: Journal of Organic Chemistry (1991), 56(24), 6773-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:20706
GI



I



II

AB The scope and limitations of the reaction of α'-nucleofuge α,β-unsatd. ketones, e.g., CH2:CHCOCH2R (R = Br, Cl, MeSO3,

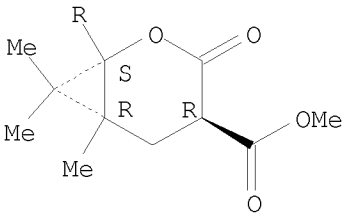
OAC), with sodium di-Me malonate was systematically studied. The substrates with good nucleofuges (halides, mesylate) give cyclopropanols, e.g., I, upon reaction with malonate anion by way of a conjugate Favorskii reaction. In reactions with substrates containing the poorer nucleofuge (acetoxy) conjugate addition proceeded without entering the Favorskii manifold. Concerning the mechanism of the Favorskii reaction, it is suggested that the loss of the nucleofuge occurs to give a 2-oxyallyl cation, but that disrotatory ring closure is facile and the only products observed result from nucleophilic trapping of cyclopropanones to yield cyclopropanols in fair to good yield. The structure of some adducts, including I and II, were determined by x-ray crystal anal.

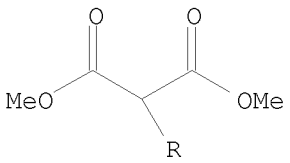
IT 136856-89-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136856-89-8 CAPLUS

CN Propanedioic acid, [4-(methoxycarbonyl)-6,7,7-trimethyl-3-oxo-2-oxabicyclo[4.1.0]hept-1-yl]-, dimethyl ester, (1α,4α,6α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.





L6 ANSWER 20 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:81505 CAPLUS

DOCUMENT NUMBER: 114:81505

ORIGINAL REFERENCE NO.: 114:13905a,13908a

TITLE: Isochroman derivatives. IX. Syntheses on the basis of 1-bromoisochroman

AUTHOR(S): Samodurova, A. G.; Markaryan, E. A.

CORPORATE SOURCE: Inst. Tonkoi Org. Khim., Yerevan, USSR

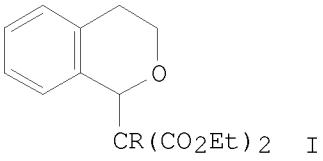
SOURCE: Armyanskii Khimicheskii Zhurnal (1990), 43(5), 332-6
CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 114:81505

GI



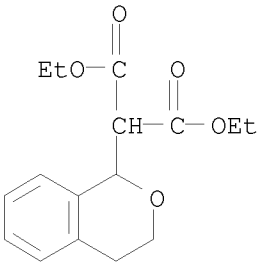
I

AB Bromination of isochroman by Br2-CCl4 activated by ultrasound gave 82.1% o-BrCH2CH2C6H4CHO (I) which was treated with CuCN to give 91.6% 1-cyanoisochroman. The latter was hydrogenated over Ni/Re or reduced by NaBH4 to give 76.1 and 71.6% 1-(aminomethyl)isochroman, resp. 1-Bromoisochroman was treated with RNaC(CO2Et)2 (R = H, Pr) to give 77.5 and 16.5% isochromans I.

IT 82584-04-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation-saponification of)

RN 82584-04-1 CAPLUS

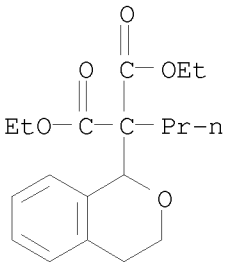
CN Propanedioic acid, (3,4-dihydro-1H-2-benzopyran-1-yl)-, diethyl ester (9CI) (CA INDEX NAME)



IT 131947-06-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 131947-06-3 CAPLUS

CN Propanedioic acid, (3,4-dihydro-1H-2-benzopyran-1-yl)propyl-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 21 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:158530 CAPLUS

DOCUMENT NUMBER: 112:158530

ORIGINAL REFERENCE NO.: 112:26803a,26806a

TITLE: Reactions of dicarbonyl(η5-

cyclopentadienyl)iron(II) complexes of two cyclic enol ethers with selected nucleophiles

AUTHOR(S): Booysen, Jozua F.; Bredenkamp, Martin W.; Holzapfel, Cedric W.

CORPORATE SOURCE: Dep. Chem., Rand Afrikaans Univ., Johannesburg, 2000, S. Afr.

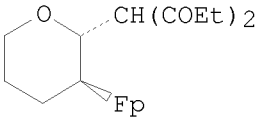
SOURCE: Synthetic Communications (1989), 19(7-8), 1449-62
CODEN: SYNCAV; ISSN: 0039-7911

DOCUMENT TYPE: Journal

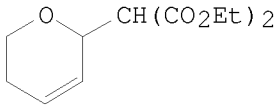
LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:158530

GI



I



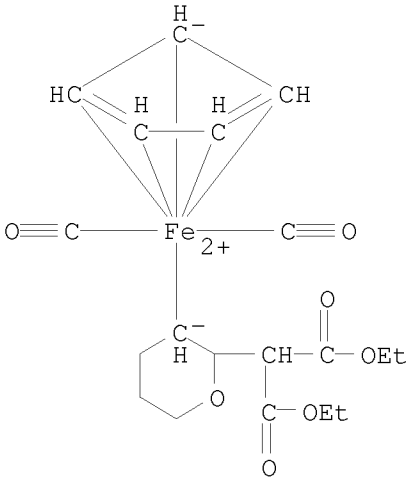
II

AB Dicarbonyl(η5-cyclopentadienyl)iron(II) complexes of 2,3-dihydrofuran and 3,4-dihydro-2H-pyran rapidly react with carbanionic nucleophiles. The adducts of certain nucleophiles, such as the anion of di-Et malonate, readily isomerize to ring opened products. Ligand exchange reactions and polymerization compete with the nucleophilic addition reactions of neutral nucleophiles such as enol ethers and indole. Thus, reaction of pyraniron complex with anion of di-Et malonate in THF gave 78% iron complex I [Fp = (η5-cyclopentadienyl)Fe(CO)2] which on demetalation with Br2 in THF gave 35% pyran II.

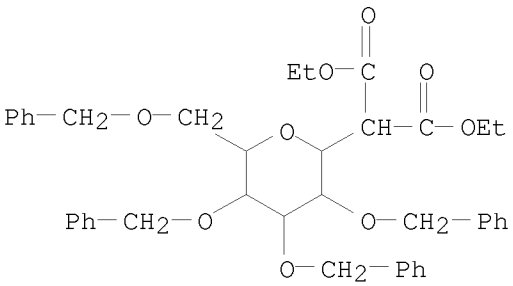
IT 126076-59-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demetalation of)

RN 126076-59-3 CAPLUS

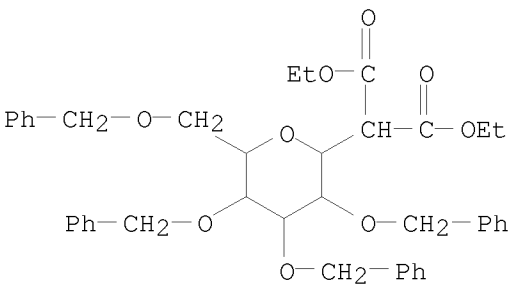
CN Iron, dicarbonyl(η5-2,4-cyclopentadien-1-yl)[2-[2-ethoxy-1-(ethoxycarbonyl)-2-oxoethyl]tetrahydro-2H-pyran-3-yl]-, stereoisomer (9CI) (CA INDEX NAME)



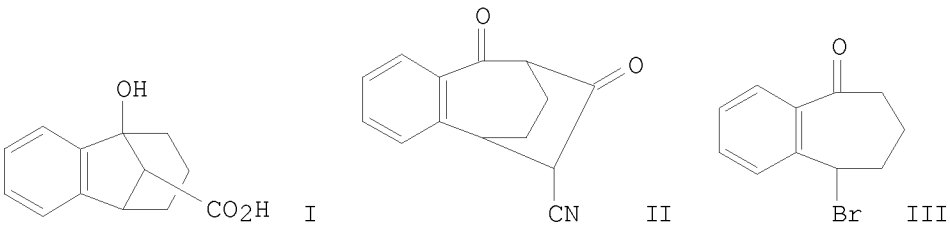
L6 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:56460 CAPLUS
DOCUMENT NUMBER: 112:56460
ORIGINAL REFERENCE NO.: 112:9715a,9718a
TITLE: Epimerization of α- to β-C-glucopyranosides under mild basic conditions
AUTHOR(S): Allevi, Pietro; Anastasia, Mario; Ciuffreda, Pierangela; Fiecchi, Alberto; Scala, Antonio
CORPORATE SOURCE: Fac. Med., Univ. Milan, Milan, I-20133, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (7), 1275-80
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:56460
AB A number of β-C-glucopyranosides having an activated methylene or methine group bonded to the anomeric carbon were obtained in high yield from the corresponding α-isomers by simple base-catalyzed equilibration at room temperature
IT 52921-16-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(anomerization of)
RN 52921-16-1 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



IT 52921-17-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)
RN 52921-17-2 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-β-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



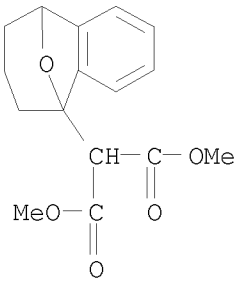
L6 ANSWER 23 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:457107 CAPLUS
DOCUMENT NUMBER: 111:57107
ORIGINAL REFERENCE NO.: 111:9683a,9686a
TITLE: Some aspects of the chemistry of benzosuberone: novel synthesis of the 5,9-methano-5H-benzocycloheptene and 6,9-ethano-5H-benzocycloheptene ring systems
AUTHOR(S): Omar, Mahmoud T.; Proctor, George R.; Scopes, David I. C.
CORPORATE SOURCE: Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, G1 1XL, UK
SOURCE: Journal of Chemical Research, Synopses (1988), (12), 383
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:57107
GI



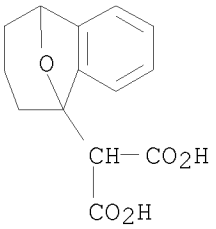
AB Bridged benzosuberans I and II were prepared from benzosuberone III. III was treated with NCCH2CO2Et, NaH, and 15-crown-5 followed by acidification to give I. The same reaction without acidification gave II.

IT 121725-25-5P 121725-50-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 121725-25-5 CAPLUS
CN Propanedioic acid, (6,7,8,9-tetrahydro-5,9-epoxy-5H-benzocyclohepten-5-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 121725-50-6 CAPLUS
CN Propanedioic acid, (6,7,8,9-tetrahydro-5,9-epoxy-5H-benzocyclohepten-5-yl)- (9CI) (CA INDEX NAME)

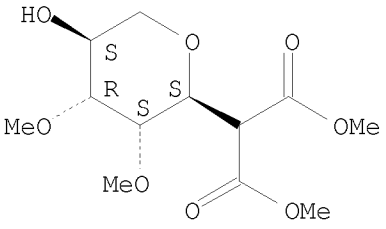


L6 ANSWER 24 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:611352 CAPLUS
DOCUMENT NUMBER: 109:211352
ORIGINAL REFERENCE NO.: 109:34979a,34982a
TITLE: Highly stereoselective total synthesis of β-ribofuranosylmalonate
AUTHOR(S): Katagiri, Nobuya; Akatsuka, Hidenori; Haneda, Toru; Kaneko, Chikara; Sera, Akira
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Journal of Organic Chemistry (1988), 53(23), 5464-70
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:211352

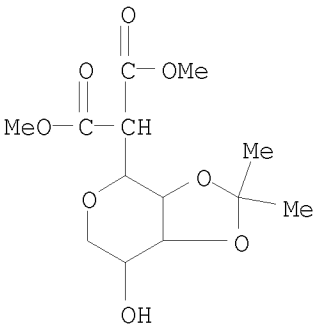
AB β-Ribofuranosylmalonates, prospective synthons for a variety of C-nucleosides, were prepared stereoselectively through the high-pressure Diels-Alder reaction of furan with dialkyl (acetoxymethylene)malonate, followed by reductive retrograde aldol C-C bond fission of the diol derived from the adduct.

IT 115479-58-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 115479-58-8 CAPLUS
CN Propanedioic acid, (2,3-di-O-methyl-α-lyxopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

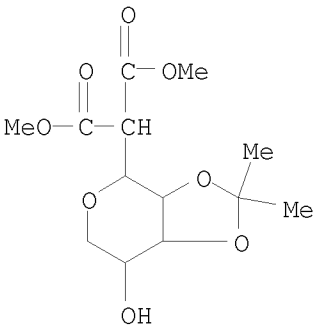
Absolute stereochemistry.



IT 117269-43-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to ribofuranosyl C-glycoside)
RN 117269-43-9 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-β-ribopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

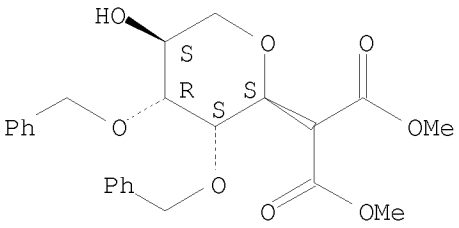


IT 117269-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 117269-40-6 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



IT 115479-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
RN 115479-61-3 CAPLUS
CN Propanedioic acid, [2,3-bis-O-(phenylmethyl)-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

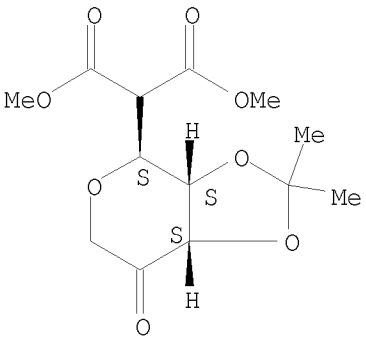
Absolute stereochemistry.



IT 117269-42-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 117269-42-8 CAPLUS

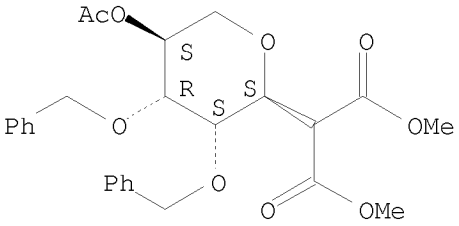
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-β-erythro-pentopyranos-4-ulos-1-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



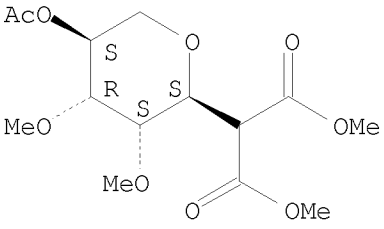
IT 115479-63-5P 115493-91-9P 117269-41-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 115479-63-5 CAPLUS
CN Propanedioic acid, [4-O-acetyl-2,3-bis-O-(phenylmethyl)-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



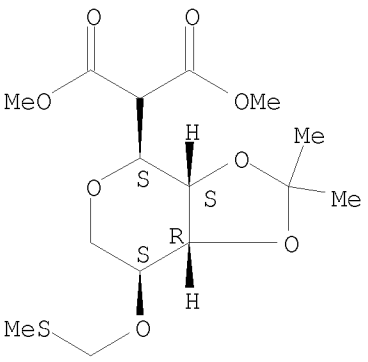
RN 115493-91-9 CAPLUS
CN Propanedioic acid, (4-O-acetyl-2,3-di-O-methyl-α-lyxopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

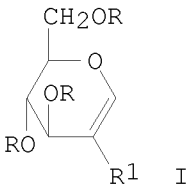


RN 117269-41-7 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-4-O-[(methylthio)methyl]-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

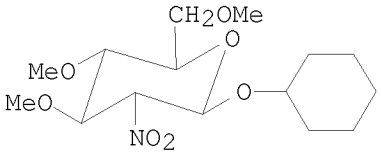
Absolute stereochemistry.



L6 ANSWER 25 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:590676 CAPLUS
DOCUMENT NUMBER: 109:190676
ORIGINAL REFERENCE NO.: 109:31579a,31582a
TITLE: 2-Nitroglycals. Preparation and nucleophilic addition reactions
AUTHOR(S): Holzapfel, C. W.; Marais, C. F.; Van Dyk, M. S.
CORPORATE SOURCE: Chem. Dep., Rand Afrikaans Univ., Johannesburg, 2000, S. Afr.
SOURCE: Synthetic Communications (1988), 18(1), 97-114
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:190676
GI



I



II

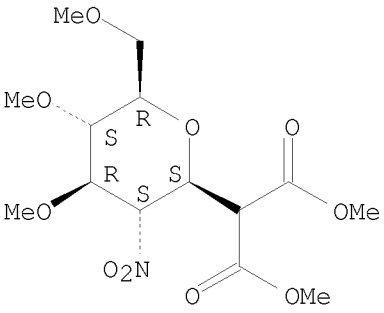
AB Nitroglycals I (R = Ac, PhCO, PhCH2, Me; R1 = NO2) were prepared by treating I (R = as above, R1 = H) with NO2+.BF4- in DME followed by a base (DBN or Et3N). I (R = PhCH2, Me; R1 = NO2) also underwent stereoselective Michael reaction with a number of nucleophiles. Thus, cyclohexanol was treated with TlOEt in DME and then with I (R = Me, R1 = NO2), followed by Me2NCH2CH2NMe2 to give 63% of the cyclohexyl deoxytrimethylnitroglucopyran oside II.

IT 117153-48-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

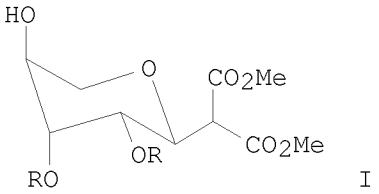
RN 117153-48-7 CAPLUS

CN Propanedioic acid, (2-deoxy-3,4,6-tri-O-methyl-2-nitro-β-D-glucopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 26 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:473790 CAPLUS
DOCUMENT NUMBER: 109:73790
ORIGINAL REFERENCE NO.: 109:12373a,12376a
TITLE: Diels-Alder reaction of dimethyl acetoxymethylenemalonate with 3,4-dialkoxyfurans and the utility of its adducts in the stereospecific synthesis of lyxopyranosyl C-glycosides
AUTHOR(S): Katagiri, Nobuya; Akatsuka, Hidenori; Haneda, Toru; Kaneko, Chikara
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chemistry Letters (1987), (11), 2257-60
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:73790
GI



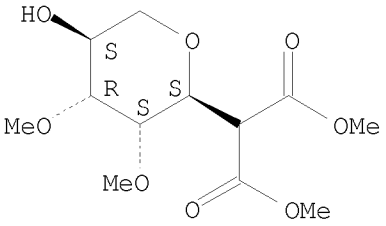
I

AB Di-Me lyxopyranosylmalonates (I; R = Me, PhCH2) were synthesized in a stereospecific manner from the adducts obtained from Diels-Alder reaction of 3,4-dialkoxyfurans and di-Me (acetoxymethylene)malonate, through retrograde aldol C-C bond fission under reductive conditions as a key step.

IT 115479-58-8P 115479-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

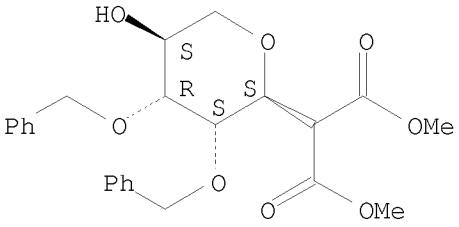
RN 115479-58-8 CAPLUS
CN Propanedioic acid, (2,3-di-O-methyl-α-lyxopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



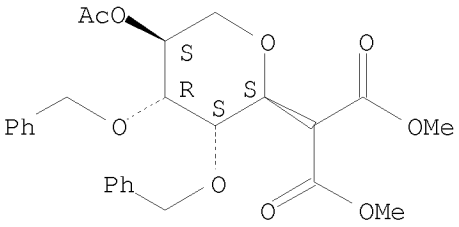
RN 115479-61-3 CAPLUS
CN Propanedioic acid, [2,3-bis-O-(phenylmethyl)-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



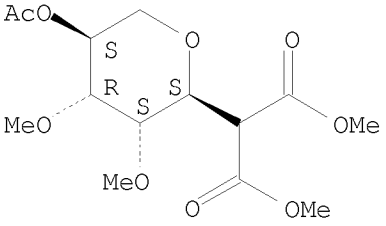
IT 115479-63-5P 115493-91-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 115479-63-5 CAPLUS
CN Propanedioic acid, [4-O-acetyl-2,3-bis-O-(phenylmethyl)-α-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



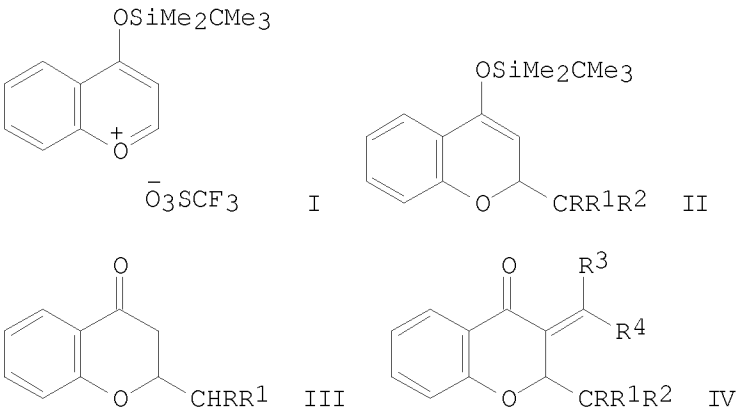
RN 115493-91-9 CAPLUS
CN Propanedioic acid, (4-O-acetyl-2,3-di-O-methyl-α-lyxopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 27 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:422811 CAPLUS
DOCUMENT NUMBER: 109:22811
ORIGINAL REFERENCE NO.: 109:3893a,3896a
TITLE: Reaction of a 4-(tert-butyldimethylsiloxy)-1-benzopyrylium salt with enol silyl ethers and active methylenes
AUTHOR(S): Iwasaki, Hideharu; Kume, Takashi; Yamamoto, Yohsuke; Akiba, Kinya
CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan
SOURCE: Tetrahedron Letters (1987), 28(50), 6355-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:22811
GI

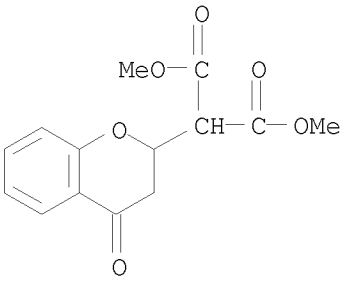


AB Butyldimethylsiloxybenzopyrylium salt I was prepared in situ from chromone and F3CSO3SiMe2CMe3 and I reacted with enol silyl ethers, ketene silyl acetals and active methylene compds to give 2-substituted butyldimethylsiloxybenzopyrans II or III (R = H, Me, Ph, CO2Me, cyano; R1 = H, Me, COCHMe2, cyano, CO2Me, Bz, CO2Et; R2 = H, COCHMe2, COEt, Ac, COC6H4Me-4, CO2Me) in 80-98% yields. II (R = R1 = H, R2 = cyano; R = R1 = Me, R2 = CO2Me) were treated with ClCOCH2CH2CO2Et and CH2:N+(Et)2Cl- to give chromanones IV (R = R1 = H, R2 = cyano, R3 = OH, R4 = CH2CH2CO2Et; R = R1 = Me, R2 = CO2Me, R3 = R4 = H).

IT 115085-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 115085-89-7 CAPLUS

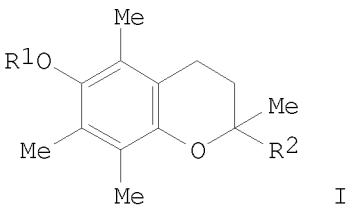
CN Propanedioic acid, (3,4-dihydro-4-oxo-2H-1-benzopyran-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 28 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:204495 CAPLUS
DOCUMENT NUMBER: 108:204495
ORIGINAL REFERENCE NO.: 108:33601a,33604a
TITLE: Preparation of halochroman derivatives as intermediates for vitamin E
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., USA
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62178581	A	19870805	JP 1987-13291	19870122 <--
US 4752646	A	19880621	US 1986-932970	19861102 <--
EP 235510	A2	19870909	EP 1987-100383	19870114 <--
EP 235510	A3	19870916		
EP 235510	B1	19890308		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
AT 41151	T	19890315	AT 1987-100383	19870114 <--
DK 8700331	A	19870724	DK 1987-331	19870121 <--
US 4806661	A	19890221	US 1988-146551	19880121 <--
US 4824971	A	19890425	US 1988-146550	19880121 <--

PRIORITY APPLN. INFO.:
US 1986-821590 A 19860123
US 1986-932970 A3 19861102
EP 1987-100383 A 19870114
OTHER SOURCE(S): CASREACT 108:204495; MARPAT 108:204495
GI



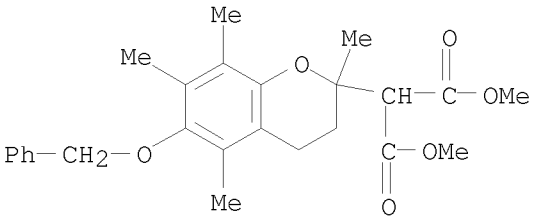
I

AB Halochroman derivs. I [R1 = Me, labile HO-protecting group; R2 = halo, 2-propenyl, CH(CO2R3)2, (CH2)3CHMe(CH2)3CHMe(CH2)3CHMe2; R3 = lower alkyl) were prepared by treating I (R2 = HO, lower alkoxy) with hydrohalo acids preferably at -30 to +30° in inert solvents or treating I (R2 =

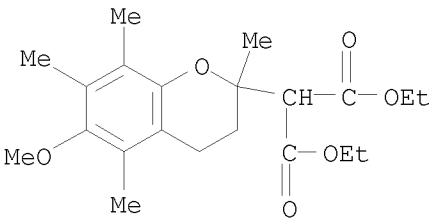
halo) with R4MgX (R4 = R2, except for halo) preferably at -100 to +0° or with R4M (M = alkali metal) preferably at -30 to -30°. Thus, treating 10 g I (R1 = PhCH2, R2 = MeO) with HCl in hexane-Et2O in the presence of CaCl2 at -5 to +10° for 1 h and stirring the mixture at room temperature for 2 h gave 10.2 g (purity 66%) I (R2 = Cl).

IT 114341-60-5P 114341-64-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for vitamin E)

RN 114341-60-5 CAPLUS
CN Propanedioic acid, [3,4-dihydro-2,5,7,8-tetramethyl-6-(phenylmethoxy)-2H-1-benzopyran-2-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

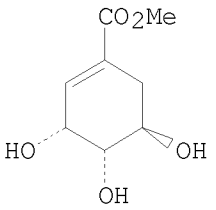


RN 114341-64-9 CAPLUS
CN Propanedioic acid, (3,4-dihydro-6-methoxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-, diethyl ester (9CI) (CA INDEX NAME)

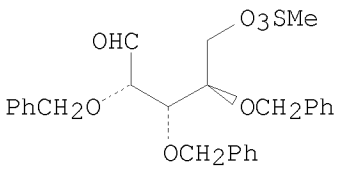


L6 ANSWER 29 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

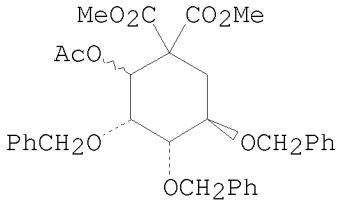
ACCESSION NUMBER: 1988:112870 CAPLUS
DOCUMENT NUMBER: 108:112870
ORIGINAL REFERENCE NO.: 108:18509a,18512a
TITLE: Synthesis of methyl (-)-shikimate from D-lyxose
AUTHOR(S): Tadano, Kinichi; Ueno, Yoshihide; Iimura, Youichi; Suami, Tetsuo
CORPORATE SOURCE: Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan
SOURCE: Journal of Carbohydrate Chemistry (1987), 6(2), 245-57
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:112870
GI



I



II



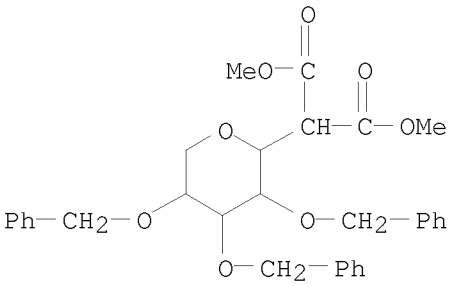
III

AB The key reaction in the synthesis of Me (-)-shikimate (I) from D-lyxose was a one-step construction of the cyclohexane ring by simultaneous C-C bond formation of both terminal carbons of a L-lyxose derived synthon II with the methylene carbon of di-Me malonate. The cyclization products III were transformed to some derivs. of shikimic acid.

IT 96290-93-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 96290-93-6 CAPLUS

CN Propanedioic acid, [2,3,4-tris-O-(phenylmethyl)-D-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 30 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:75724 CAPLUS

DOCUMENT NUMBER: 108:75724

ORIGINAL REFERENCE NO.: 108:12547a,12550a

TITLE: Syntheses of pseudo-α-D-glucopyranose and pseudo-β-L-altropyranose from L-arabinose

AUTHOR(S): Tadano, Kinichi; Kameda, Yukiaki; Iimura, Youichi; Suami, Tetsuo

CORPORATE SOURCE: Fac. Sci. Technol., Keio Univ., Yakohama, 223, Japan

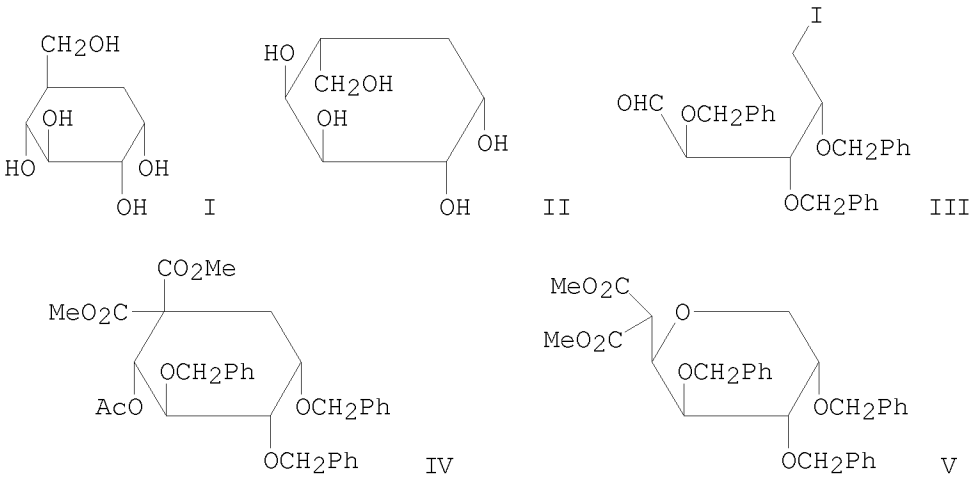
SOURCE: Journal of Carbohydrate Chemistry (1987), 6(2), 231-44
CODEN: JCACDM; ISSN: 0732-8303

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:75724

GI

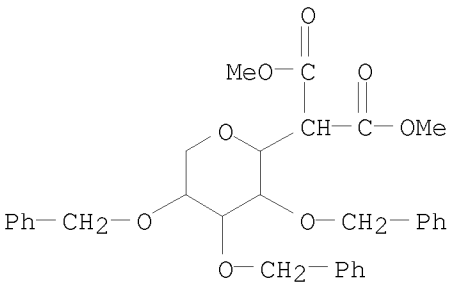


AB In the preparation of the title compds. I and II, iododeoxyarabinose (III) was the key intermediate, which was obtained in 7 steps from L-arabinose. The reaction of III with di-Me malonate under basic conditions provided a tetrahydroxylated cyclohexane-1,1-dicarboxylate IV and a C-glycoside of β-L-arabinopyranose V. From IV, I and II were prepared by (1) thermal demethoxycarbonylation, (2) LiAlH4 reduction, (3) hydroboration of the resulting 1-hydroxymethyl-1-cyclohexene derivative followed by H2O2 treatment, and (4) removal of the protecting groups.

IT 112709-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112709-64-5 CAPLUS

CN Propanedioic acid, [2,3,4-tris-O-(phenylmethyl)-β-L-arabinopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 31 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:554607 CAPLUS

DOCUMENT NUMBER: 107:154607

ORIGINAL REFERENCE NO.: 107:24893a,24896a

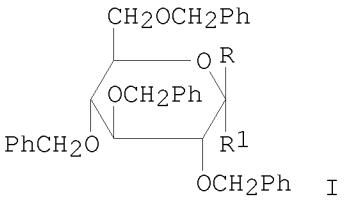
TITLE: C-Glucopyranosyl derivatives from readily available 2,3,4,6-tetra-O-benzyl-α-D-glucopyranosyl chloride

AUTHOR(S): Allevi, Pietro; Anastasia, Mario; Ciuffreda, Pierangela; Fiecchi, Alberto; Scala, Antonio

CORPORATE SOURCE: Fac. Med. Chir., Univ. Milano, Milan, I-20133, Italy

SOURCE: Journal of the Chemical Society, Chemical

Communications (1987), (2), 101-2
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:154607
GI



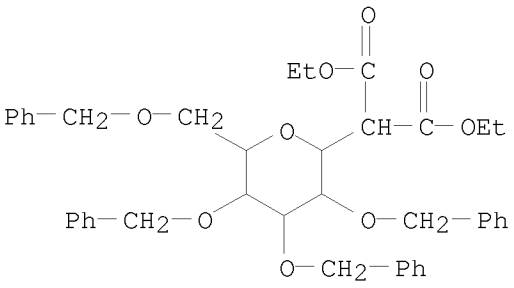
I

AB Treatment of the title glucopyranosyl chloride (I; R = H, R1 = Cl) with EtO2CCH:C(OSiMe3)OEt, CH2:C(OSiMe3)Ph, CH2:C(OSiMe3)C6H4Cl-p, CH2:C(OSiMe3)CMe3, or CH2:C(OSiMe3)Me in CH2Cl2 10 min at room temperature in the dark in the presence of silver triflate gave C-glucopyranosyl derivs. with α-configuration [I; R = H, R1 = CH(CO2Et)2, CH2COPh, CH2COC6H4Cl-p, CH2COCMe3, CH2COMe] in 75-88% yields. Similar reaction with m-(MeO)2C6H4 gave the β-anomer [I; R = 2,4-(MeO)2C6H3] in 40% yield.

IT 52921-16-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and debenzylation followed by acetylation of)

RN 52921-16-1 CAPLUS

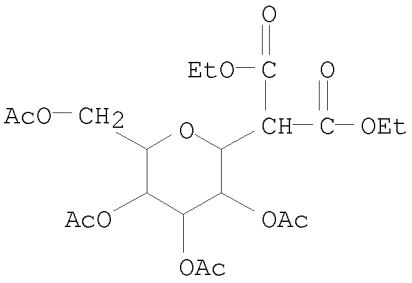
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



IT 52950-02-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 52950-02-4 CAPLUS

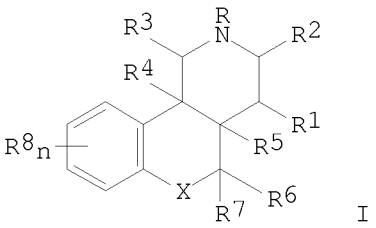
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 32 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:477780 CAPLUS
DOCUMENT NUMBER: 107:77780
ORIGINAL REFERENCE NO.: 107:12805a,12808a
TITLE: Hexahydro-[1]-benzo(pyrano and -thiopyrano)[4,3-c]pyridines useful as serotonin-2 blocking agents
INVENTOR(S): Schneider, Josef A.
PATENT ASSIGNEE(S): Ciba-Geigy Corp., USA
SOURCE: U.S., 16 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4666916	A	19870519	US 1985-796348	19851108 <--
EP 222703	A1	19870520	EP 1986-810496	19861031 <--
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 43610	A2	19871130	HU 1986-4631	19861106 <--
HU 196409	B	19881128		
DK 8605330	A	19870509	DK 1986-5330	19861107 <--
FI 8604548	A	19870509	FI 1986-4548	19861107 <--
NO 8604455	A	19870511	NO 1986-4455	19861107 <--
AU 8664950	A	19870514	AU 1986-64950	19861107 <--
AU 598765	B2	19900705		
ZA 8608486	A	19870624	ZA 1986-8486	19861107 <--
DD 252376	A5	19871216	DD 1986-296073	19861107 <--
JP 62142180	A	19870625	JP 1986-264915	19861108 <--

PRIORITY APPLN. INFO.: US 1985-796348 A 19851108
OTHER SOURCE(S): CASREACT 107:77780; MARPAT 107:77780
GI



I

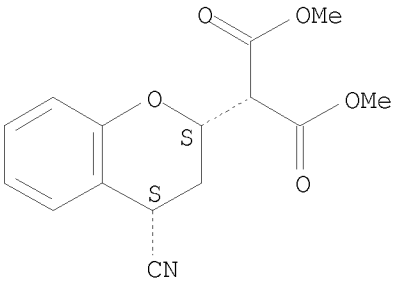
AB The title compds. [I; R = H, alkyl, alkenyl, alkynyl, aroylalkyl, aralkyl;

R1 = H, (un)substituted alkyl; R2-R7 = H, alkyl; R8 = H, alkoxy, acyloxy, halo, alkyl, CF3, alkylenedioxy; X = O, S; n = 0-3] were prepared for treatment of gastrointestinal, cardiovascular, and central nervous system disorders. (±)-[4R, 4AS, 10bR]-7-bromo-4-hydroxymethyl-1,3,4,4a,5,10b-hexahydro-9-methoxy-2-methyl-2H-[1]benzopyrano[4,3-c]pyridine (preparation given) was mesylated and the mesylate displaced with ethanethiolate anion to give (±)-[4R,4aS,10bR]-7-bromo-4-(ethylthiomethyl)-1,3,4,4a,5,10b-hexahydro-9-methoxy-2-methyl-2H-[1]benzopyrano[4,3-c]pyridine (II). II inhibited binding at the serotonin-2 receptor with an IC50 of 2.2 + 10-8M. Capsules were prepared containing II 10.0, lactose 207, modified starch 80.0, and Mg stearate 3.0 g/1,000 capsules.

IT 109543-01-3P 109543-09-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive cyclization of, benzopyranopyridinecarboxylate derivative by)

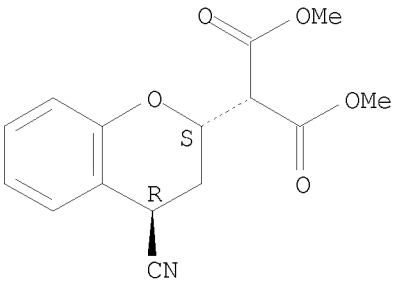
RN 109543-01-3 CAPLUS
CN Propanedioic acid, (4-cyano-3,4-dihydro-2H-1-benzopyran-2-yl)-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



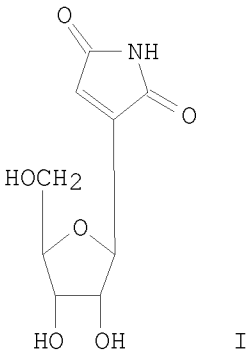
RN 109543-09-1 CAPLUS
CN Propanedioic acid, (4-cyano-3,4-dihydro-2H-1-benzopyran-2-yl)-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:214228 CAPLUS
DOCUMENT NUMBER: 106:214228
ORIGINAL REFERENCE NO.: 106:34777a,34780a
TITLE: New entry to the C-glycosidation by means of carbenoid displacement reaction. Its application to the synthesis of showdomycin
AUTHOR(S): Kametani, Tetsuji; Kawamura, Kuniaki; Honda, Toshio
CORPORATE SOURCE: Inst. Med. Chem., Hoshi Univ., Tokyo, 142, Japan

SOURCE: Journal of the American Chemical Society (1987), 109(10), 3010-17
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:214228
GI

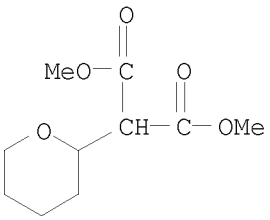


I

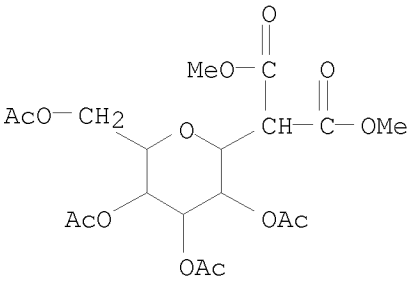
AB A novel and stereoselective carbon-carbon bond-forming reaction at the anomeric center of carbohydrates has been developed by means of a carbenoid displacement reaction with Ph thioglycosides. This reaction is suggested to proceed via the oxonium ion intermediates and has the following advantages: (i) the preferential participation of a carbenoid with a sulfur atom can restrict the reaction site; (ii) the reaction can be carried out under neutral reaction condition; and (iii) the introduction of various functionalities can be accomplished by manipulation of the organosulfur groups of the products. This synthetic strategy was successfully applied to the synthesis of antitumor agent, (+)-showdomycin (I) and would provide a general route to the other C-glycosides.

IT 107961-17-1P 107961-19-3P 107961-20-6P
107961-21-7P 107961-22-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

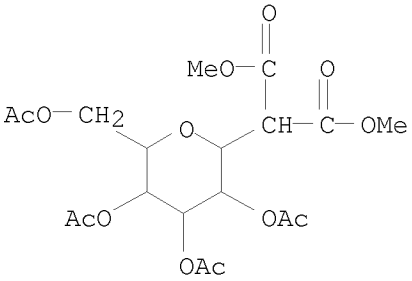
RN 107961-17-1 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2H-pyran-2-yl)-, 1,3-dimethyl ester (CA INDEX NAME)



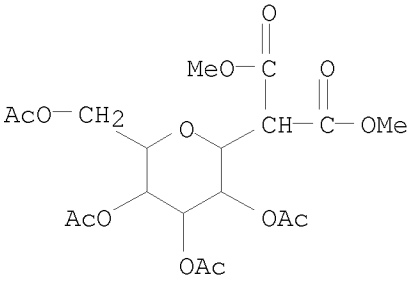
RN 107961-19-3 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 107961-20-6 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-mannopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

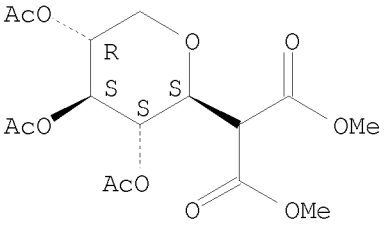


RN 107961-21-7 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-α-D-galactopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 107961-22-8 CAPLUS
CN Propanedioic acid, (2,3,4-tri-O-acetyl-β-D-arabinopyranosyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

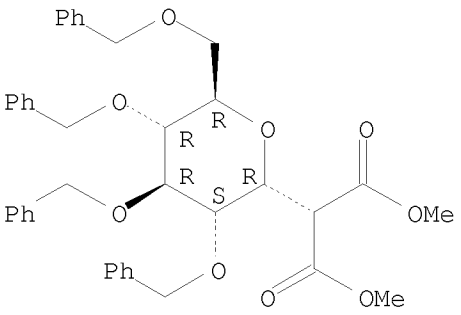


L6 ANSWER 34 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:422859 CAPLUS
DOCUMENT NUMBER: 103:22859
ORIGINAL REFERENCE NO.: 103:3791a,3794a
TITLE: C-Glycosidation of pyridyl thioglycosides
AUTHOR(S): Stewart, Andrew O.; Williams, Robert M.
CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
SOURCE: Journal of the American Chemical Society (1985), 107(14), 4289-96
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:22859

AB Ag(I) activation of pyridyl thioglycosides in the presence of carbon nucleophiles yield C-glycosides under mild conditions with high stereoselectivity. Pyridyl thioglycosides of suitably protected carbohydrates represent stable precursors to structurally complex C-glycosides. Per-O-benzyl-1-(2-pyridylthio)-D-glucose, per-O-benzyl-1-(2-pyridylthio)-D-ribose, and 1-(2-pyridylthio)-2,3-O-isopropylidene-5-O-(tert-butyldiphenylsilyl)-D-ribofuranose were prepared, and their reactions with a variety of both electron-rich aroms. and silyl enol ethers of carbonyl compds. are reported. The glucose substrate shows a general α selectivity. However, the ribosyl substrates exhibit high α,β selectivity which reveal a large dependence upon the specific nucleophile.

IT 96689-83-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 96689-83-7 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 35 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:203800 CAPLUS
DOCUMENT NUMBER: 102:203800
ORIGINAL REFERENCE NO.: 102:31937a,31940a
TITLE: Synthesis of methyl (-)-shikimate from D-lyxose
AUTHOR(S): Suami, Tetsuo; Tadano, Kinichi; Ueno, Yoshihide; Iimura, Youichi
CORPORATE SOURCE: Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan
SOURCE: Chemistry Letters (1985), (1), 37-40
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English

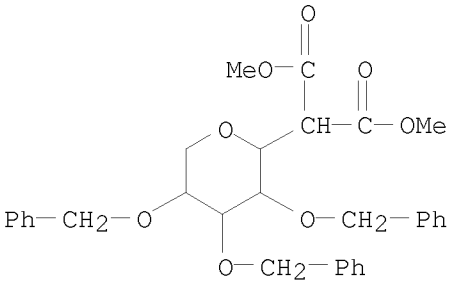
OTHER SOURCE(S): CASREACT 102:203800

AB Natural Me (-)-shikimate has been synthesized from D-lyxose, employing a double C-C bond formation of 2,3,4-tri-O-benzyl-5-O-mesyl-D-lyxose with a dianion of CH2(CO2Me)2 as a key reaction.

IT 96290-93-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 96290-93-6 CAPLUS

CN Propanedioic acid, [2,3,4-tris-O-(phenylmethyl)-D-lyxopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 36 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:95925 CAPLUS

DOCUMENT NUMBER: 102:95925

ORIGINAL REFERENCE NO.: 102:15105a,15108a

TITLE: Synthesis of optically active pseudo-α-D-glucose and pseudo-β-L-altrose

AUTHOR(S): Suami, Tetsuo; Tadano, Kinichi; Kameda, Yukiaki; Iimura, Youichi

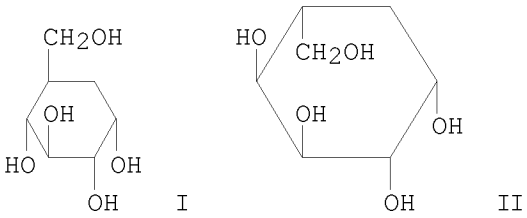
CORPORATE SOURCE: Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan

SOURCE: Chemistry Letters (1984), (11), 1919-22
CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

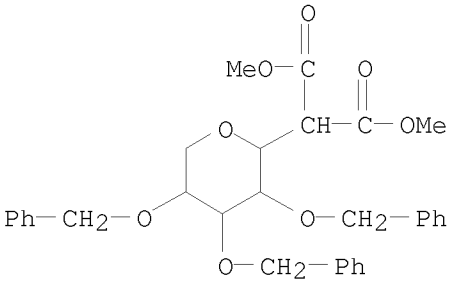


AB Pseudo-α-D-glucose (I) and pseudo-β-L-altrose (II) were synthesized from L-arabinose with the cyclization of 2,3,4-tri-O-benzyl-5-deoxy-5-iodo-L-arabinose with CH2(CO2Me)2 in the presence of NaH as a key reaction.

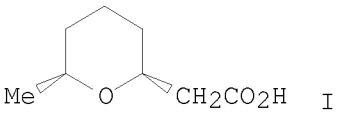
IT 94898-35-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 94898-35-8 CAPLUS

CN Propanedioic acid, [2,3,4-tris-O-(phenylmethyl)-L-arabinopyranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 37 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:612331 CAPLUS
DOCUMENT NUMBER: 99:212331
ORIGINAL REFERENCE NO.: 99:32667a,32670a
TITLE: Synthesis of the civet constituent cis-(6-methyltetrahydropyran-2-yl)acetic acid
AUTHOR(S): Bates, Hans Aaron; Deng, Ping Nan
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794, USA
SOURCE: Journal of Organic Chemistry (1983), 48(24), 4479-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

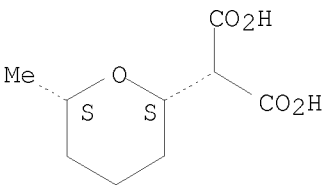
AB The civet constituent cis-(6-methyltetrahydropyran-2-yl)acetic acid (I) was prepared In the key step, trans-2-chloro-6-methyltetrahydropyran reacted with NaCH(CO2Me)2 with inversion to afford di-Me cis-2-methyltetrahydropyran-2-yl)malonate. Hydrolysis and decarboxylation of the latter compound provided I.

IT 87393-75-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 87393-75-7 CAPLUS

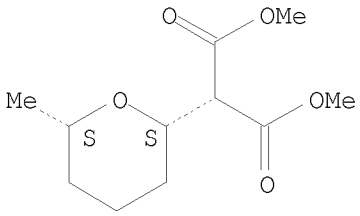
CN Propanedioic acid, (tetrahydro-6-methyl-2H-pyran-2-yl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



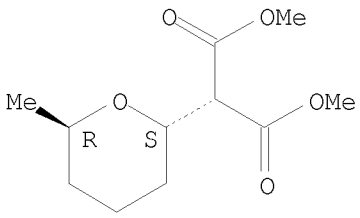
IT 87393-74-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)
RN 87393-74-6 CAPLUS
CN Propanedioic acid, (tetrahydro-6-methyl-2H-pyran-2-yl)-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 87393-76-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87393-76-8 CAPLUS
CN Propanedioic acid, (tetrahydro-6-methyl-2H-pyran-2-yl)-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



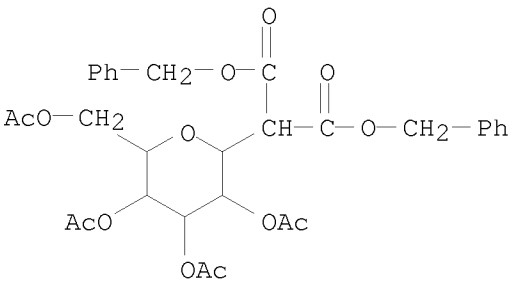
L6 ANSWER 38 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:139581 CAPLUS
DOCUMENT NUMBER: 98:139581
ORIGINAL REFERENCE NO.: 98:21195a,21198a
TITLE: Effect of aryl substituents on the kinetics of inactivation of glycosidases by glycosylmethylaryltriazenes: examination of the suicide nature of these inactivations
AUTHOR(S): Sinnott, Michael L.; Tzotzos, George T.; Marshall, Susan E.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Bristol, Bristol, BS8 1TS, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1982), (12), 1665-70
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The inactivation of the Mg2+-free form of the gene lacZ β-galactosidase of Escherichia coli at 25° by various [(β-D-galactopyranosyl)methyl]aryltriazenes resembles the spontaneous, rather than the acid-catalyzed, decomposition of

alkylaryltriazenes in that both the maximum 1st-order rate constant, and the 2nd-order rate constant, are governed by a neg. β1g value at pH 7.0 and 8.0. Less extensive measurements for the β-xylosidase of Penicillium wortmanni and [(β-D-xylopyranosyl)methyl]aryltriazenes give a similar result. Although the decomposition of the 2-(β-D-galactopyranosyl)ethyl compds. in aqueous solution is 5- to 10-fold faster than their lower homologs, β-galactosidase inactivation is 3- to 13-fold slower. [(β-D-Galactopyranosyl)methyl](p-nitrophenyl)triazene does not inactivate the lectin, RCA ricin.

IT 85114-15-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and catalytic hydrogenolysis of)

RN 85114-15-4 CAPLUS

CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



L6 ANSWER 39 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:582753 CAPLUS

DOCUMENT NUMBER: 97:182753

ORIGINAL REFERENCE NO.: 97:30593a,30596a

TITLE: Stereospecific synthesis of the phosphono analogs of α- and β-D-glucose 1-phosphate

AUTHOR(S): Nicotra, Francesco; Ronchetti, Fiamma; Russo, Giovanni

CORPORATE SOURCE: Fac. Sci., Univ. Milan, Milan, 20133, Italy

SOURCE: Journal of Organic Chemistry (1982), 47(23), 4459-62
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

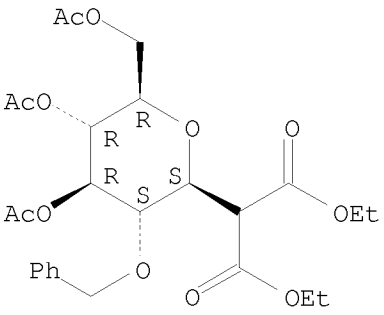
AB (1-Deoxy-β-D-glucopyranosyl)methanephosphonic acid was prepared by treating 2,6-anhydro-1-bromo-1-deoxy-3,4,5,7-tetra-O-acetyl-D-glycero-D-gluco-heptitol with P(OEt)3 followed by deethylation of the resulting di-Et (glucopyranosyl)methanephosphonate and deacetylation with ion-exchange resin. The α-glucopyranosyl analog was prepared from 2,3,4,6-tetra-O-benzyl-D-glucose by Wittig reaction with H2C:PPh3, mercuricyclization, bromodemercuration, Arbuzov reaction, and removal of the protecting groups.

IT 82933-05-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

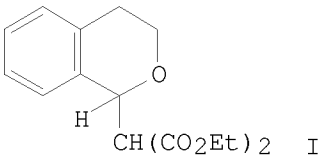
RN 82933-05-9 CAPLUS

CN Propanedioic acid, [3,4,6-tri-O-acetyl-2-O-(phenylmethyl)-β-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



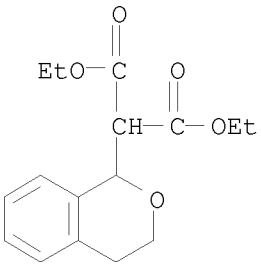
L6 ANSWER 40 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:491389 CAPLUS
DOCUMENT NUMBER: 97:91389
ORIGINAL REFERENCE NO.: 97:15234h,15235a
TITLE: Reactivity of isocoumarins. V. Reaction of 1-ethoxyisochroman with active methylene compounds
AUTHOR(S): Ishikawa, Tadataka; Yamato, Masatoshi
CORPORATE SOURCE: Fac. Pharm. Sci., Okayama Univ., Okayama, 700, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1982), 30(5), 1594-601
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:91389
GI



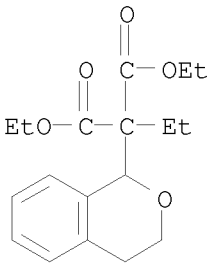
I

AB Active methylene compds. (di-Et malonate, α-tetralone, dimedone, acetylacetone, malononitrile, and diketene) reacted with 1-ethoxyisochroman to give the corresponding 1-substituted isochroman derivs., e.g., I. When I was treated with sodium ethoxide or potassium tert-butoxide, Et 1,4-dihydro-2-naphthoate, Et 1,2-dihydro-2-naphthoate, and Et 2-naphthoate were obtained. However, the reaction of 2-(1-isochromanyl)cyclohexanone with potassium tert-butoxide gave 9-formyl-1,2,3,4-tetrahydroanthracene and 1,2,3,4.9,10-hexahydroanthracene. The conversion mechanisms of 1-substituted isochromans into naphthalenes and 1,2,3,4-tetrahydroanthracenes are proposed.

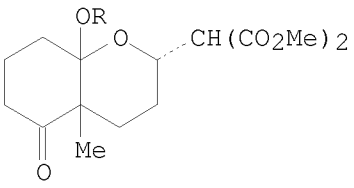
IT 82584-04-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with sodium ethoxide or potassium tert-butoxide, naphthoates from)
RN 82584-04-1 CAPLUS
CN Propanedioic acid, (3,4-dihydro-1H-2-benzopyran-1-yl)-, diethyl ester (9CI) (CA INDEX NAME)



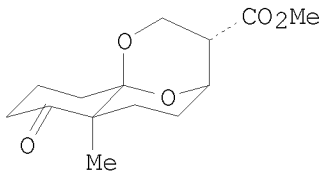
IT 82584-12-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82584-12-1 CAPLUS
CN Propanedioic acid, (3,4-dihydro-1H-2-benzopyran-1-yl)ethyl-, diethyl ester (9CI) (CA INDEX NAME)



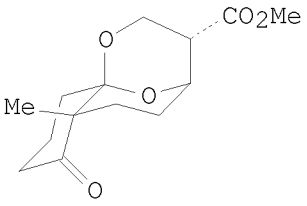
L6 ANSWER 41 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:593146 CAPLUS
DOCUMENT NUMBER: 91:193146
ORIGINAL REFERENCE NO.: 91:31106h,31107a
TITLE: Synthetic methods. 15. A fragmentative access to macrolides: (5-E,9-E)-6-methyl-5,8-undecadien-11-olide
AUTHOR(S): Shibuya, Masayuki; Jaisli, Fritz; Eschenmoser, Albert
CORPORATE SOURCE: Fac. Pharm. Sci., Tokushima Univ., Tokushima, Japan
SOURCE: Angewandte Chemie (1979), 91(8), 672-3
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



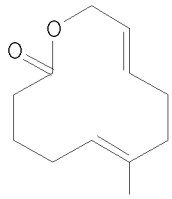
I



II



III



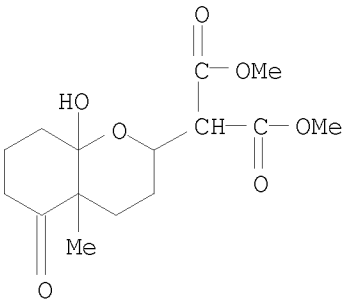
IV

AB Michael addition of acrolein with 2-methyl-1,2-cyclohexanedione with subsequent condensation with CH2(CO2Me)2 gave I (R = H), which, after conversion into I (R = Me), was subjected to successive LiAlH4 reduction, intramol. transacetalization and oxidation to give a 3:1 mixture of II and III, whose configuration was established by 13C-NMR. II and III were converted into the corresponding amidinium carboxylates, which, upon fusion, gave the title compound IV.

IT 70968-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methanolysis of)

RN 70968-63-7 CAPLUS

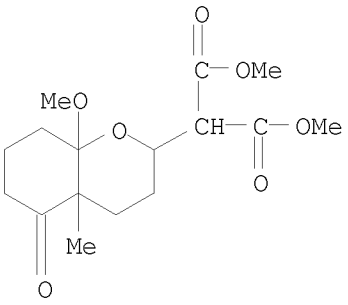
CN Propanedioic acid, (octahydro-8a-hydroxy-4a-methyl-5-oxo-2H-1-benzopyran-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



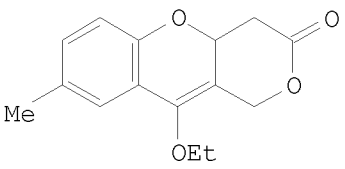
IT 70968-64-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 70968-64-8 CAPLUS

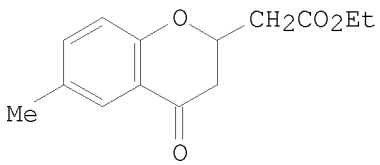
CN Propanedioic acid, (octahydro-8a-methoxy-4a-methyl-5-oxo-2H-1-benzopyran-2-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



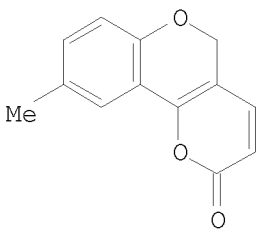
L6 ANSWER 42 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:601383 CAPLUS
DOCUMENT NUMBER: 87:201383
ORIGINAL REFERENCE NO.: 87:31883a,31886a
TITLE: An exploration of a synthetical route to the pyrano[4,3-b][1]benzopyran nucleus of the fungal metabolite fulvic acid; rearrangements in chromanone derivatives
AUTHOR(S): Dean, Francis M.; Murray, Stephen; Smith, Dennis A.
CORPORATE SOURCE: Robert Robinson Lab., Univ. Liverpool, Liverpool, UK
SOURCE: Journal of Chemical Research, Synopses (1977), (9), 230-1
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

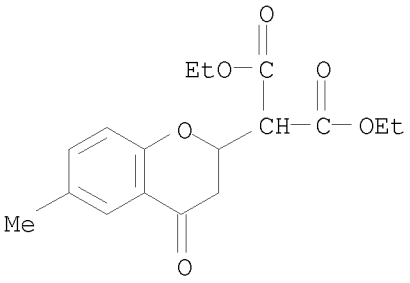


II

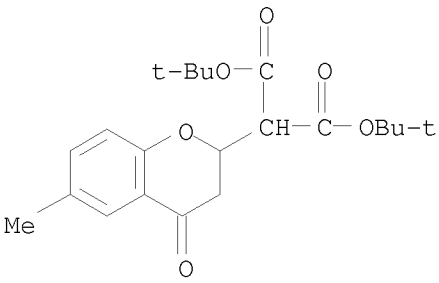


III

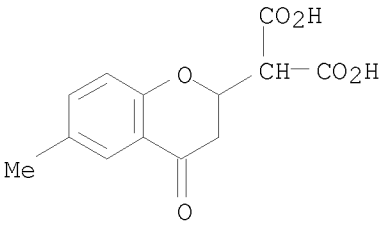
AB The pyrano[4,3,-b][1]benzopyran derivative I was prepared from the chromanone ester II by sequential treatment with BF3.Et2O-HC(OEt)3, NaBH4, and NaH in distilling C6H6. Several title rearrangements are discussed, including one generating the pyrano[3,2-c][1]-benzopyran derivative III.
IT 64802-30-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64802-30-8 CAPLUS
CN Propanedioic acid, (3,4-dihydro-6-methyl-4-oxo-2H-1-benzopyran-2-yl)-, diethyl ester (9CI) (CA INDEX NAME)



IT 64802-40-0P 64802-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in pyranobenzopyran derivative preparation)
RN 64802-40-0 CAPLUS
CN Propanedioic acid, (3,4-dihydro-6-methyl-4-oxo-2H-1-benzopyran-2-yl)-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

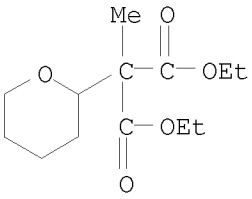


RN 64802-41-1 CAPLUS
CN Propanedioic acid, (3,4-dihydro-6-methyl-4-oxo-2H-1-benzopyran-2-yl)- (9CI) (CA INDEX NAME)



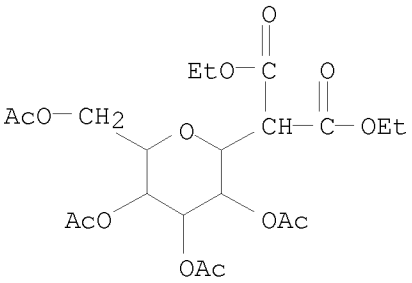
L6 ANSWER 43 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:496358 CAPLUS
DOCUMENT NUMBER: 83:96358
ORIGINAL REFERENCE NO.: 83:15117a,15120a
TITLE: Addition reaction of the organozinc derivative of ethyl methylbromomalonate to β-acetylenic compounds. Applications to the synthesis of lactones and lactams
AUTHOR(S): Bertrand, Marie T.; Courtois, Gilles; Miginiac, Leone
CORPORATE SOURCE: Lab. Synth. Org., Univ. Poitiers, Poitiers, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1975), 280(15), 999-1002
CODEN: CHDCAQ; ISSN: 0567-6541

DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 83:96358
GI For diagram(s), see printed CA Issue.
AB The Reformatskii reaction of HC.tplbond.CCHRC(OH)R1R2 with MeC(CO2Et)2Br (I) gave six δ-valerolactones (II; R = H, Me; R1 = H, Me; R2 = H, Me, Ph, CHMe2). I reacted with Zn and HC.tplbond.CCH2CHRNHEt (R = H, Ph) to give mixts. of CH2:C[C(CO2Et)2Me]CH2CHRNHEt and δ-lactams (III).
IT 56518-06-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56518-06-0 CAPLUS
CN Propanedioic acid, methyl(tetrahydro-2H-pyran-2-yl)-, diethyl ester (9CI) (CA INDEX NAME)



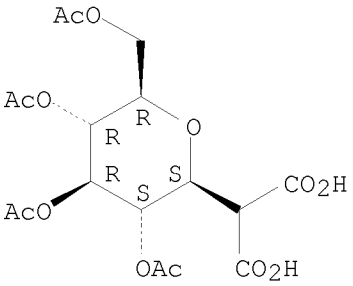
L6 ANSWER 44 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:413713 CAPLUS
DOCUMENT NUMBER: 81:13713
ORIGINAL REFERENCE NO.: 81:2215a,2218a
TITLE: Carbanions in carbohydrate chemistry. Synthesis of C-glycosyl malonates
AUTHOR(S): Hanessian, Stephen; Pernet, Andre G.
CORPORATE SOURCE: Dep. Chem., Univ. Montreal, Montreal, QC, Can.
SOURCE: Canadian Journal of Chemistry (1974), 52(8, Pt. 1), 1266-79
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 81:13713
AB The condensation of 2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl bromide with sodio di-Et malonate (I) led to crystalline di-Et 2-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)malonate. The corresponding dibenzyl ester was used for the preparation of crystalline β-D-glucopyranosylmalonic acid and β-D-glucopyranosyl acetic acid derivs. The anomeric configuration in these C-glycosides was determined by a chemical correlation. With 2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl chloride and I, the major product was a 1,2-O-acetal derivative The condensation of 2,3,4,6-tetra-O-benzyl-α-D-glucopyranosyl bromide with I was conducted with, and without added bromide ion and the mechanistic implications of the results are discussed. C-Glycosides were also prepared in the D-mannofuranose series and their transformation into the D-lyxofuranose series (anomeric mixture) is described. The utility of NMR shift reagents, and an apparent differential complexation by Eu(DPM)3 (DPM = dipivalomethanato) and Eu(FOD)3-d27 (FOD = 6,6,7,7,8,8,8-heptafluoro-2,2-dimethyloctanedionato) is demonstrated.
IT 34010-27-0P 34010-28-1P 34049-06-4P
52921-16-1P 52921-17-2P 52921-52-5P
52921-53-6P 52950-02-4P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 34010-27-0 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)

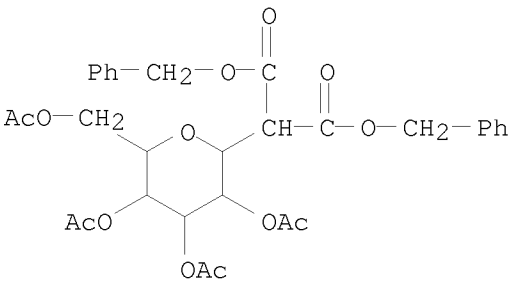


RN 34010-28-1 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

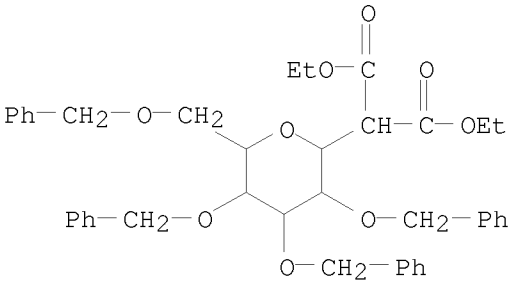
Absolute stereochemistry.



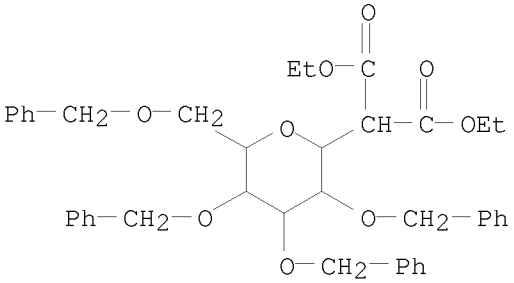
RN 34049-06-4 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



RN 52921-16-1 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-α-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

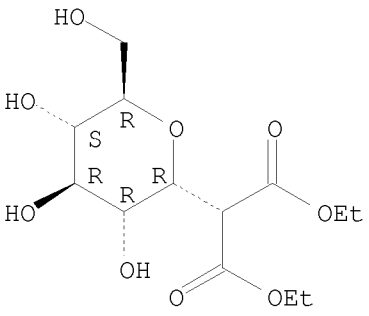


RN 52921-17-2 CAPLUS
CN Propanedioic acid, [2,3,4,6-tetrakis-O-(phenylmethyl)-β-D-glucopyranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



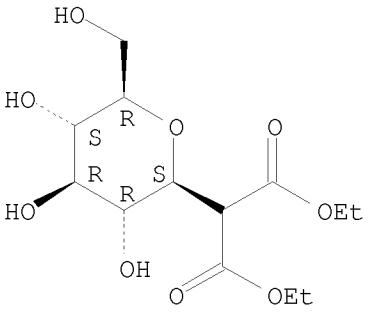
RN 52921-52-5 CAPLUS
CN Propanedioic acid, α-D-glucopyranosyl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

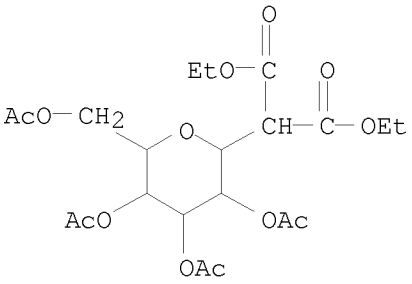


RN 52921-53-6 CAPLUS
CN Propanedioic acid, β-D-glucopyranosyl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

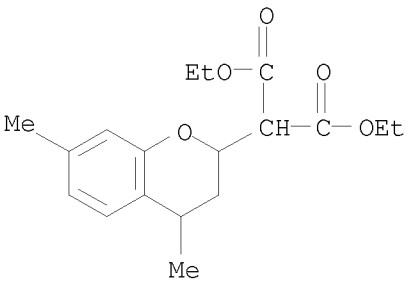


RN 52950-02-4 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)

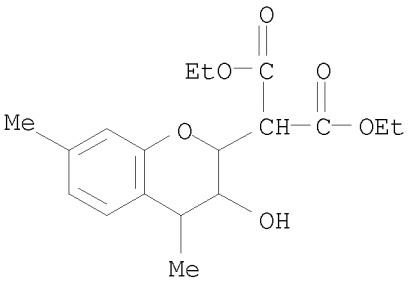


L6 ANSWER 45 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:491904 CAPLUS
DOCUMENT NUMBER: 79:91904
ORIGINAL REFERENCE NO.: 79:14923a,14926a
TITLE: Aromatic precursors in trichothecene synthesis. Addition of lithioethyl acetate to a pyrylium salt
AUTHOR(S): Goldsmith, David J.; Helmes, C. Tucker, Jr.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, USA
SOURCE: Synthetic Communications (1973), 3(3), 231-5
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB With a view to the synthesis of trichothecene compds., various synthetic pathways were explored. Thus, hydrogenation of 4,7-dimethylcoumarin gave 4,7-dimethyl-2-chromanol which on condensation with CH2(CO2Et)2 gave the diester I [R = CH(CO2Et)2, X = H2]. Hydrolysis and decarboxylation of the diester gave I (R = CH2CO2H, X = H2) which on reduction gave the alc. I (R = CH2CH2OH, X = H2) (II). Barton nitrite photolysis of II did not give the keto alc. I (R = CH2CH2OH, X = O) but the disproportionation compound I (R = CH2CHO, X = H2). Knoevenagel condensation of CH2(CO2Et)2 with 4,7-dimethyl-2,3-chromandiol gave ≤20% I [R = CH(CO2Et)2, X = H, OH] and III. Reaction of 7-methoxy-4-chromone with MeLi in HClO4 gave the pyrylium salt (IV) which on treatment with MeCO2CH2CH2Li gave 68% (V). Reductive hydrocarboration of V with pyridine/borane gave the diol (VI).
IT 43015-45-8P 43015-50-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 43015-45-8 CAPLUS
CN Propanedioic acid, (3,4-dihydro-4,7-dimethyl-2H-1-benzopyran-2-yl)-,

diethyl ester (9CI) (CA INDEX NAME)



RN 43015-50-5 CAPLUS
CN Propanedioic acid, (3,4-dihydro-3-hydroxy-4,7-dimethyl-2H-1-benzopyran-2-yl)-, diethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 46 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:405331 CAPLUS
DOCUMENT NUMBER: 79:5331
ORIGINAL REFERENCE NO.: 79:903a,906a
TITLE: (Carboxymethyl)penicillins
INVENTOR(S): Burton, George; Davies, John Sydney; Hubbard, Ann Frances
PATENT ASSIGNEE(S): Beecham Group Ltd.
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2249085	A1	19730412	DE 1972-2249085	19721006 <--
GB 1424186	A	19760211	GB 1971-46929	19720908 <--
US 3926955	A	19751216	US 1972-291798	19720925 <--
JP 48044295	A	19730626	JP 1972-98900	19721002 <--
JP 55025193	B	19800704		

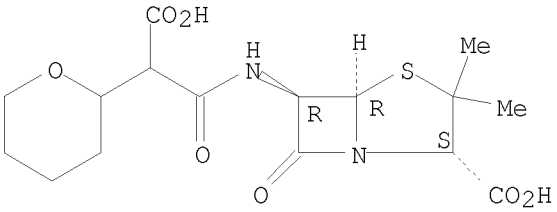
PRIORITY APPLN. INFO.: GB 1971-46929 A 19711008
GI For diagram(s), see printed CA Issue.
AB Eight title compds. (I, n = 1, 3, 4, or 5) and(or) their Na or Ca salts, useful as bactericides, feed additives, and drugs for the treatment of mastitis, were prepared by reaction of 6-aminopenicillanic acid (II) or its benzyl ester with HO2CCHRCOX (X = OH, Cl, or OCH2Ph) or their chlorides and optionally hydrogenation. Thus, cyclo-propanemalonic acid was

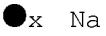
successively refluxed with SOCl2 in Et2O in the presence of DMF 2 hr and with PhCH2OH in Et2O 2 hr to give 49% benzyl hydrogen cyclopropanemalonate (III). III was successively treated with SOCl2 1 hr at 70° and with II in aqueous NaOH, NaHCO3, and Me2CO 2 hr at room temperature to give 77% Na
[(benzyloxycarbonyl)cyclopropylmethyl]penicillin (IV). IV was hydrogenated over Pd/CaCO3 in H2O to give 80% I (R = cyclopropyl) Ca salt.

IT 49574-89-2P 49574-90-5P 49574-91-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

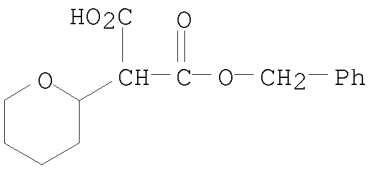
RN 49574-89-2 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[carboxy(tetrahydro-2H-pyran-2-yl)acetyl]amino]-3,3-dimethyl-7-oxo-, sodium salt, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



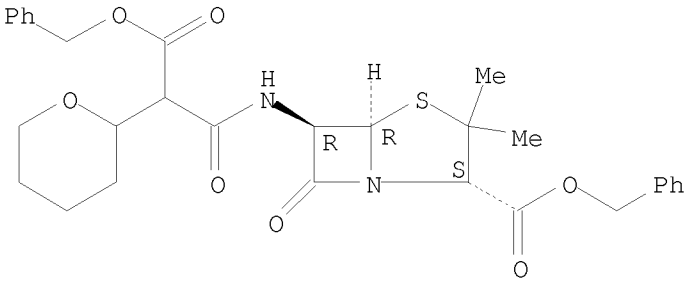


RN 49574-90-5 CAPLUS
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)-, mono(phenylmethyl) ester (9CI) (CA INDEX NAME)

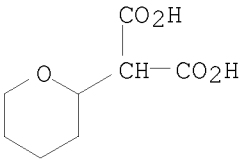


RN 49574-91-6 CAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[1,3-dioxo-3-(phenylmethoxy)-2-(tetrahydro-2H-pyran-2-yl)propyl]amino]-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-(2α,5α,6β)]- (9CI) (CA INDEX NAME)

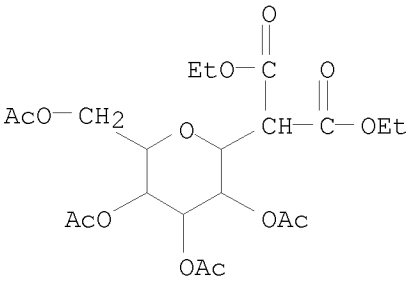
Absolute stereochemistry.



IT 49574-99-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with phenyldiazomethane)
RN 49574-99-4 CAPLUS
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)

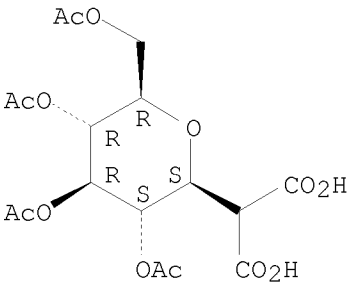


L6 ANSWER 47 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:530030 CAPLUS
DOCUMENT NUMBER: 75:130030
ORIGINAL REFERENCE NO.: 75:20539a,20542a
TITLE: Carbanions in carbohydrate chemistry. New synthesis of C-glycosyl compounds
AUTHOR(S): Hanessian, S.; Pernet, A. G.
CORPORATE SOURCE: Dep. Chem., Univ. Montreal, Montreal, QC, Can.
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1971), (14), 755-6
CODEN: CCJDAO; ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 75:130030
GI For diagram(s), see printed CA Issue.
AB Reaction of α-D-glucopyranosyl bromide tetraacetate with NaH-CH2(CO2Et)2 or NaH-CH2(CO2CH2Ph)2 followed by hydrogenolysis (Pd-C) gave β-D-glucopyranosylmalonic acid tetraacetate, which was decarboxylated (refluxing AcOH) to give β-D-glucopyranosylacetic acid tetracetate; a Hunsdiecker reaction then gave the bromide (I), which was solvolyzed (DMF-NaOAc) to give 1,3,4,5,7-penta-O-acetyl-2,6-anhydro-D-glycero-D-gulo-heptitol (II).
IT 34010-27-0P 34010-28-1P 34049-06-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34010-27-0 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-, diethyl ester (9CI) (CA INDEX NAME)

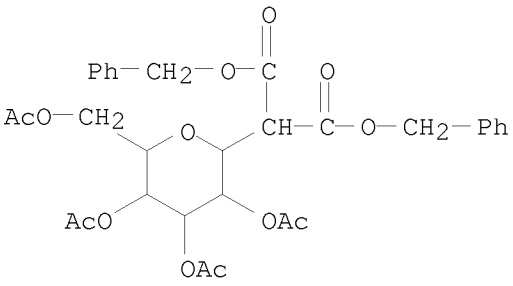


RN 34010-28-1 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 34049-06-4 CAPLUS
CN Propanedioic acid, (2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



L6 ANSWER 48 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:3136 CAPLUS
DOCUMENT NUMBER: 68:3136
ORIGINAL REFERENCE NO.: 68:623a
TITLE: Behavior of ketone toward α-methoxy hemiacetal halides related to tetrahydropyran and to carbohydrates
AUTHOR(S): Hurd, Charles D.; Richardson, Arturo Jorge
CORPORATE SOURCE: Northwestern Univ., Evanston, IL, USA
SOURCE: Journal of Organic Chemistry (1967), 32(11), 3516-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

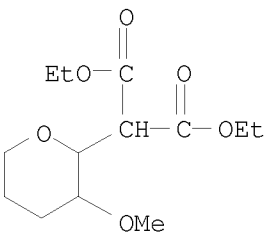
OTHER SOURCE(S): CASREACT 68:3136

AB A 3-methoxyl substituent in tetrahydropyran-2-yl chloride inhibits reactivity of the halogen toward ketene and $ZnCl_2$ more than does a 3-acetoxyl group. Both give rise to a γ-lactone. A trace of γ-lactone results also from interaction of ketene ($ZnCl_2$) with tetra-O-methyl-D-glucopyranosyl bromide. Related structures in the tetrahydropyran series which showed a neg. response with ketene are discussed and alternate syntheses of many of them included. 13 references.

IT 14194-89-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14194-89-9 CAPLUS

CN 2H-Pyran-2-malonic acid, tetrahydro-3-methoxy-, diethyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 49 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:464090 CAPLUS

DOCUMENT NUMBER: 67:64090

ORIGINAL REFERENCE NO.: 67:12031a,12034a

TITLE: Naphthalidylmalonic ester

AUTHOR(S): Suszko, Jerzy; Kinastowski, Stefan

CORPORATE SOURCE: Polska Akad. Nauk, Poznan, Pol.

SOURCE: Roczniki Chemii (1967), 41(3), 523-8
CODEN: ROCHAC; ISSN: 0035-7677

DOCUMENT TYPE: Journal

LANGUAGE: Polish

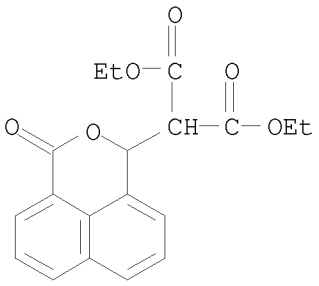
GI For diagram(s), see printed CA Issue.

AB Synthesis of the title compound and the proof of its structure was reported. K (or Na) naphthaldehyde carboxylate (I) was used as the starting material. Naphthaldehyde carboxylic acid reacted in its desmotropic cyclic form as 3-hydroxynaphthalide (II). Thus, a solution of 5 g. II in 20 ml. aqueous KOH (prepared from 1.4 g. KOH) was filtered and treated with 4 g. KCl to give 4 g. I (M = K), which was added portionwise with cooling to 3.5 g. oxalyl chloride in 20 ml. benzene. The mixture was left 48 hrs. at room temperature, refluxed 15 min., and filtered hot to remove KCl. The filtrate afforded III, m. 230° (C_6H_6). When concentrated the mother liquors, after separation of III, yielded (IV), m. 145° (1:1 benzene-ligroine). A solution of 7.5 g. diethylmalonate in 30 ml. anhydrous benzene and 0.21 g. powdered Na was kept 12 hrs. and treated with 2 g. III, stirred 15 min. and filtered. The filtrate was washed, dried, and evaporated to give dinaphthalidylmalonic ester, m. 175° (alc.). The alc. mother liquors were boiled (C) and filtered to give naphthalidylmalonic di-Et ester (V), m. 110°. An improved synthesis of V was carried out: a solution of I (M = Na) (prepared from 2 g. II in 10 ml. aqueous NaOH containing 0.4 g. NaOH) was treated with 2.5 ml. diethyl malonate and 5 ml. EtOH. Two drops piperidine was added, the mixture saturated with CO_2, kept 5 hrs. at

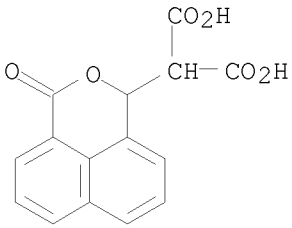
room temperature, and inoculated with V to induce crystallization of V. Saturation was
repeated at 24-hr. intervals during one week until 1.5 g. V septd. Hydrolysis of 1 g. V with 0.8 g. NaOH in 20 ml. water, during 13 hrs. at room temperature, followed by acidification at 0° with dilute HCl, gave naphthalidylmalonic acid, m. 145° (decomposition), which decomposed in vacuo at 144° to give naphthalidylacetic acid VI, m. 158°. Condensation of IV with diethyl malonate, carried out as described above for III, led to a mixture of V and IX, m. 272°. The formation of IX was explained by the reaction sequence IV → VII → VIII → IX.

IT 7090-54-2P 14955-56-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 7090-54-2 CAPLUS
CN 1H,3H-Naphtho[1,8-cd]pyran-1-malonic acid, 3-oxo-, diethyl ester (8CI) (CA INDEX NAME)



RN 14955-56-7 CAPLUS
CN 1H,3H-Naphtho[1,8-cd]pyran-1-malonic acid, 3-oxo- (8CI) (CA INDEX NAME)



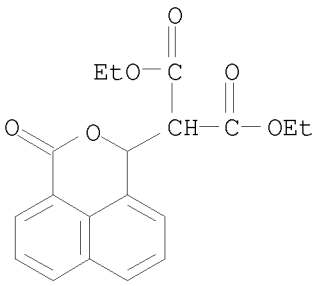
L6 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:465365 CAPLUS
DOCUMENT NUMBER: 65:65365
ORIGINAL REFERENCE NO.: 65:12146d-e
TITLE: Structure and properties of naphthalic acid derivatives
AUTHOR(S): Suszko, J.; Kinastowski, S.
CORPORATE SOURCE: A. Mickiewicz Univ., Poznan
SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1966), 14(5), 277-80
CODEN: BAPCAQ; ISSN: 0001-4095
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Naphthaloyl chloride (I) with Na diethyl malonate gives II and Et

naphthaloylacetate (III) (CA 31, 17946). Treatment of II with Na diethylmalonate gives III, showing that III is a secondary product. The structure of II was demonstrated by ir and uv spectroscopy. The reaction of II with KOEt gave the K salt of IV. Acidification gives free IV. With FeCl3 IV gives a red color While in acid IV reverts to II. Treatment of IV with CuSO4 gives a deep green crystalline salt, m. 142-5° while the reaction of IV with BzCl gave a Bz derivative, m. 111°.

IT 7090-54-2, Malonic acid, [(8-carboxy-1-naphthyl)hydroxymethyl]-, δ-lactone, di-Et ester
(spectrum of)

RN 7090-54-2 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-malonic acid, 3-oxo-, diethyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1966:456632 CAPLUS

DOCUMENT NUMBER: 65:56632

ORIGINAL REFERENCE NO.: 65:10538b-c

TITLE: Anomalous reactions of naphthalylmalonic ester

AUTHOR(S): Suszko, J.; Kinastowski, S.

CORPORATE SOURCE: A. Mickiewicz Univ., Poznan

SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1966), 14(5), 281-4
CODEN: BAPCAQ; ISSN: 0001-4095

DOCUMENT TYPE: Journal

LANGUAGE: English

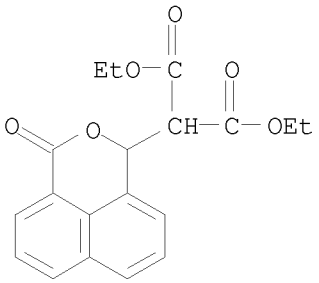
GI For diagram(s), see printed CA Issue.

AB I is reduced with 2 moles H2 and Raney Ni to give II, which can be reduced to give III and IV. Reduction of I or III with LiAlH4 gave V, m. 228°. Reduction of VI gave VII, m. 152°. Oxidation of III with CrO3 in AcOH yielded I.

IT 7090-54-2P, Malonic acid, [(8-carboxy-1-naphthyl)hydroxymethyl]-, δ-lactone, di-Et ester
RL: PREP (Preparation)
(preparation of)

RN 7090-54-2 CAPLUS

CN 1H,3H-Naphtho[1,8-cd]pyran-1-malonic acid, 3-oxo-, diethyl ester (8CI) (CA INDEX NAME)



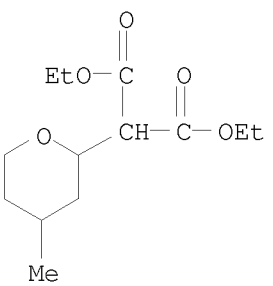
L6 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:429402 CAPLUS
DOCUMENT NUMBER: 65:29402
ORIGINAL REFERENCE NO.: 65:5445e-f
TITLE: 2- and 2,6-Substituted etrahydrofurans and tetrahydropyrans
INVENTOR(S): Hoffmann, Werner; Schneider, Kurt; Pasedach, Heinrich
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik A.-G.
SOURCE: 12 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 656115		19650524	BE	19641123 <--
PRIORITY APPLN. INFO.:			DE	19631126

AB 4-Methyl-2-methoxytetrahydropyran (260 parts), 300 parts AcCH2CO2Et, and 10 parts p-toluenesulfonic acid is refluxed 3 hrs. while the MeOH which sep. is removed to give 40% Et 2-(4-methyl,2-tetrahydropyranyl)acetoacetate, b1.5 101°, n25D 1.4520. Et 2-(2-tetrahydropyranyl)acetoacetate, b1.5 99°, n25D 1.4520, yield 45%; di-Et 2-(4-methyl-2-tetrahydroxypyranyl)malonate, b0.199°, n25D 1.4427, yield 75%; and Et 2-(2-tetrahydrofuranyl)- acetoacetate, b0.4 77°, n25D 1.4480, yield 65%, are also prepared and are intermediates for pharmaceuticals, dyes, and pesticides.

IT 6576-55-2P, Pyran-2-malonic acid, tetrahydro-4-methyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)

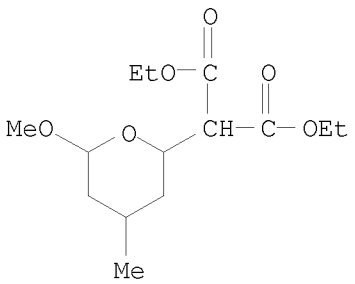
RN 6576-55-2 CAPLUS
CN Pyran-2-malonic acid, tetrahydro-4-methyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



L6 ANSWER 53 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:403933 CAPLUS
DOCUMENT NUMBER: 65:3933
ORIGINAL REFERENCE NO.: 65:691e-g
TITLE: 2-Alkyltetrahydropyrans and 2-alkyl-3,4-dihydro-2H-pyrans
INVENTOR(S): Hoffmann, Werner; Pasedach, Heinrich
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik A.-G.
SOURCE: 9 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 657537		19650415	BE	<--
PRIORITY APPLN. INFO.:			DE	19640428

GI For diagram(s), see printed CA Issue.
AB 2-Hydroxy-3,4-dihydro-2H-pyrans are treated with an equimolar amount of a compound containing an active Me, CH2, or CH group in the presence of 0.1-1 mole-% acid, such as p-MeC6H4SO3H, BF3 etherate, AlCl3, or ZnCl2, to give compds. of the general formulas I and II which can be used as chemical intermediates. Thus, a mixture of 384 parts 2-methoxy-4-methyl-3,4-dihydro-2H-pyran, 480 parts CH2(CO2Et)2, and 5 parts AlCl3 is refluxed 10 hrs. at 10-20 mm. to give 90% mixture, b0.3 114-16°, n25D 1.477, of 2-methoxy-4-methyl-6-[bis(carbethoxy)methyl]tetrahydropyran (III) and 2-[bis(carbethoxy)methyl]4-methyl-3,4-dihydro-2H-pyran (IV), III-IV ratio .apprx.10:1. Similarly, prepared are the following I and II (R, R1, b.p./mm. I, n25D I, b.p./mm. II, and n25d II given): H, Ac, 108-12°/0.6, 1.4545, 101-2°/0.8, 1.4610; Me, Ac, 106-8°/0.3, 1.4565, 92-3°/0.3, 1.4671.
IT 6263-92-9P, Pyran-2-malonic acid, tetrahydro-6-methoxy-4-methyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 6263-92-9 CAPLUS
CN Pyran-2-malonic acid, tetrahydro-6-methoxy-4-methyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



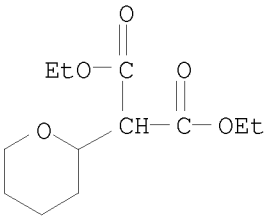
L6 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:403338 CAPLUS
DOCUMENT NUMBER: 59:3338
ORIGINAL REFERENCE NO.: 59:551e-g
TITLE: Condensation of tetrahydro-2-pyranol with active methylene compounds

AUTHOR(S): Coblentz, Michael; Royer, Jean; Dreux, Jacques
SOURCE: Bulletin de la Societe Chimique de France (1963) 310-13
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 59:3338

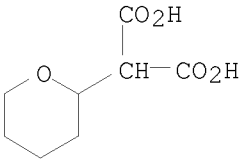
AB Tetrahydro-2-pyranol (I) and PhCH2CN in the presence of KOMe gave phenyl(tetrahydro-2-pyranyl)methane, b1 164-5°, n2D5 1.553, d25 1.052. I and PhCH2COMe gave after repeated purifications 1-phenyl-1-(tetrahydro-2-pyranyl)-2-propanone, b1 126°, n2D5 1.5215, d25 1.054; 2,4-dinitrophenylhydrazone m. 118°. I and PhCH2COPh gave 1-oxo-1,2-diphenyl-2-(tetrahydro-2-pyranyl)ethane, m. 130°; 2,4-dinitrophenylhydrazone m. 165°. I and PhCOMe gave 1-oxo-1-phenyl-2-(tetrahydro-2-pyranyl)ethane, b1 130-1°, n2D5 1.5353, d25 1.085; 2,4-dinitrophenylhydrazone m. 194°. I and PhCOEt gave after involved purifications 1-phenyl-2-(tetrahydro-2-pyranyl)propanone, b1 123°, n2D5 1.5287, d25 1.073; 2,4-dinitrophenylhydrazone m. 192.5°. I and acetylacetone gave 3-(tetrahydro-2-pyranyl)acetylacetone b12 120°, n2D5 1.4629, d25 1.046; dioxime m. 164°. I and Et acetylacetate gave Et [3-oxo-2-(tetrahydro-2-pyranyl)]acetylacetate (II), b1 97-8°, n2D5 1.4528, d25 1.069. II and aqueous KOH gave K 2-(tetrahydro-2-pyranyl)acetate; acid m. 56-7°. I and Et malonate gave Et 2-(tetrahydro-2-pyranyl)malonate, b1 110° n2D5 1.4475, d25 1.074. I and Et cyanoacetate gave Et 2-cyano-2-(tetrahydro-2-pyranyl)acetate, b1 120°, n2D5 1.4563, d25, 1.081.

IT 5468-59-7P, Pyran-2-malonic acid, tetrahydro-, diethyl ester
49574-99-4P, Pyran-2-malonic acid, tetrahydro-
RL: PREP (Preparation)
(preparation of)

RN 5468-59-7 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)

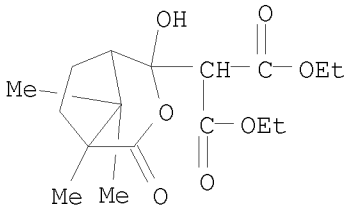


RN 49574-99-4 CAPLUS
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)

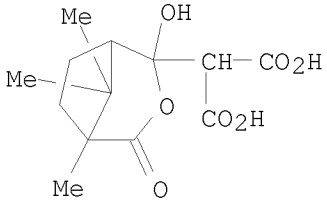


L6 ANSWER 55 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:17641 CAPLUS
DOCUMENT NUMBER: 55:17641

ORIGINAL REFERENCE NO.: 55:3462b-g
TITLE: The reaction between sodio diethylmalonate and dl-camphoric anhydride
AUTHOR(S): Eskola, Salli; Tirronen, Toivo; Kiianlinna, Kiuru
CORPORATE SOURCE: Univ. Helsinki
SOURCE: Suomen Kemistilehti B (1960), 33B, 80-2
CODEN: SUKBAJ; ISSN: 0371-4101
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB cf. Lapworth and Royle, CA 14, 2914. The reaction of NaCH(CO2Et)2 (I) and dl-camphoric anhydride (II) is known [Winzer, Ann. 257, 298 (1890)] to give diethyl camphorylmalonate (III). From the crude reaction mixture containing I was isolated a solid, m. 62-3°, soluble in Na2CO3, and giving a red color with alc. FeCl3, which was formulated as IV (R = H). The initial product formed from I and II was postulated as IV (R = CO2Et), which decarbethoxylated to IV (R = H) and also dehydrated to III. To a suspension of 13.8 g. granular Na in 300 ml. dry C6H6 cooled in ice was added slowly 96 g. CH2(CO2Et)2. After 17 hrs., 109 g. camphoric anhydride was slowly added and the mixture refluxed 200 hrs. and acidified with dilute HCl, the C6H6 layer separated and extracted once with NaHCO3 solution and several times with Na2CO3 solution Distillation of the C6H6 and excess CH2(CO2Et)2 left 18.6 g. (crude) III, m. 80-1° (Et2O and EtOH). Acidification of the Na2CO3 exts. gave IV (R = H), b0.32 155-61°; m. 62-3° (ligroine).
IT 114204-15-8P, Malonic acid, [(3-carboxy-2,2,3-trimethylcyclopentyl)dihydroxymethyl]-, δ-lactone, di-Et ester
857243-75-5P, 3-Oxabicyclo[3.2.1]octane-2-malonic acid, 2-hydroxy-5,8,8-trimethyl-4-oxo-
RL: PREP (Preparation)
(preparation of)
RN 114204-15-8 CAPLUS
CN Malonic acid, [(3-carboxy-2,2,3-trimethylcyclopentyl)dihydroxymethyl]-, δ-lactone, diethyl ester (6CI) (CA INDEX NAME)



RN 857243-75-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

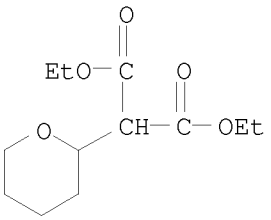


L6 ANSWER 56 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:8064 CAPLUS
DOCUMENT NUMBER: 55:8064
ORIGINAL REFERENCE NO.: 55:1593i,1594a-i,1595a-c
TITLE: Stereochemistry of manoyl oxide
AUTHOR(S): Hodges, R.; Reed, R. I.
CORPORATE SOURCE: Univ. Glasgow, UK
SOURCE: Tetrahedron (1960), 10, 71-5
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The stereochemistry of manoyl oxide (I) at C-8 was established by hydrogenolysis to 8α-hydroxylabd-13-ene (II). Electron-impact induced fission of the mol. showed that C-16 had a β-configuration and that I had the given structure. I (500 mg.) in 15 ml. dry Et2O kept 30 min. with 1 g. Li in 75 ml. liquid NH3 and excess Li destroyed with NH4Cl, the product chromatographed on 50 g. Al2O3 (activity III) and eluted with 9:1 C6H6-Et2O gave 445 mg. II, m. 99-100.5° (Kofler block, corrected) (dilute MeOH), [α]20D-1° (c 1.0, in CHCl3), ν 826 cm.-1 (Nujol), also given by hydrogenolysis of epimanoyl oxide (III) under the same conditions. Ozonolysis of II in AcOH gave 63% AcH, isolated as 2,4-dinitrophenylhydrazone. Accordingly, III as prepared by Ohloff (CA 53, 8192d) was the C-13 epimer. II (93 mg.) kept 15 hrs. at 20° with 200 ml. POCl3 in 2 ml. C5H5N, the product taken up in C5H12, filtered through Al2O3 (activity I) and distilled at 100°/0.05 mm. gave a 75:16:9 mixture of all 3 possible dehydration products, C20H34, [α]D 37.3° (c 1.3), containing labda-8(20),13-diene as the major component. The ΔMD value, 105°, was in reasonable agreement with that of 98° between sclareol and manool, corresponding to removal of one asym. center, so that C-20 in I had probably a β orientation. I (1.31 g.) and 1.25 g. OsO4 in 5 ml. C5H5N kept 48 hrs. at 0° in Et2O and the ester decomposed with H2S, the product adsorbed from C6H6 on 100 g. Al2O3 and eluted with 19:1 Et2O-MeOH, the black oily product (1.35 g.) refluxed 30 min. with 3.5 g. Pb(OAc)4 in 60 ml. C6H6 and adsorbed from C6H6 on Al2O3, eluted with 9:1 C6H6-Et2O and the colorless oily aldehyde (IV, R = CHO) (V) treated with H2NNHCONH2.HCl gave the semicarbazide, m. 225-7.5° (dilute alc.). V (169 mg.) and 39 mg. CrO3 kept 12 hrs. in 5 ml. AcOH at 20° and the acidic product taken up in C6H6, chromatographed on SiO2 gel and eluted with CHCl3 gave 72 mg. IV (R = CO2H), m. 45-7° (dilute MeOH), dried 48 hrs. at 40°/0.05 mm. to give a sample, m. 97-8°, [α]D 42° (c 0.7); Me ester, m. 83-5° (dilute MeOH), [α]D 14° (c 0.5), ν 1731, 1751 cm.-1 (CCl4). The neutral product from the CrO3 oxidation adsorbed on 20 g. Al2O3 from petr. ether (b. 60-80°) and eluted with 9:1 C6H6-Et2O yielded 21 mg. lactone (VI), m. 125-6.5° (petr. ether), [α]D 41° (c 0.8, C6H6), infrared spectrum identical with that of the authentic compound (Hinder and Stoll, CA 49, 11609b). VI was less stable than the corresponding 8-epimer and its isolation provided evidence of an 8-oxido group in I. It was decided to alter the shape of the I mol. to make it distinguishable from its C-13 epimer. NaBH4 (250 mg.) and 250 mg. 2-oxomanoyl oxide kept 2 hrs. in 15 ml. aqueous MeOH and the product refluxed 1 hr. in 4 ml. Ac2O with 500 mg. NaOAc, taken up in petr. ether and chromatographed on 25 g. Al2O3, eluted with 9:1 petr. ether-C6H6 and the product crystallized from petr. ether gave 200 mg. 2α-acetoxy-8α,13-oxidolabd-14-ene, m. 107.5-109°, [α]D 37° (c 1.5), brominated (54 mg.) with 0.85 ml. Br in CCl4 (2.9%) in 3 ml. CCl4 at 0° to give 48 mg. 2α-acetoxy-14,15-dibromo-8α, 13-oxidolabdane, m.

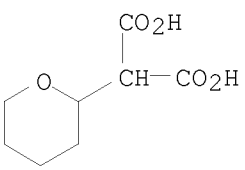
125-134°, stirred (950 mg.) 3 hrs. in Et2O with NaNH2 (from 2 g. Na) in 100 ml. liquid NH3 at -33°, the reacetylated product taken up on 100 g. Al2O3 (activity V) from petr. ether and eluted with 9:1 petr. ether-C6H6 to yield 370 mg. 2α-acetoxy-8α,13-oxidolabd-14-yne (VII), m. 115-116.5°, [α]D 12° (c 1.2), hydrolyzed to the corresponding alc. (VIII), m. 104-5° (petr. ether), [α]D 38° (c 0.8). VIII (125 mg.) in 10 ml. Me2CO oxidized with 8N CrO3/H2SO4 gave 112 mg. 8α,13-oxido-2-oxolabd-14-yne (IX), m. 98-100°, [α]D 29° (c 0.9). IX (92 mg.) and 200 mg. Cu(OAc)2 refluxed 20 min. in 2 ml. C5H5N and the product crystallized from CH2Cl2-MeOH yielded 78 mg. 15,15'-bi(8α,13-oxido-2-oxolabd-14-ynyl) (X), m. 258-60°, [α]D -40° (C 0.65), λ 232, 243, 254, 284 mμ (ε 405, 410, 310, 136, CH2Cl2). The 2 C-13 epimers of this structure had very different mol. dimensions but no steric conclusions could be drawn from an x-ray determination of the size of the crystal unit cell. The probability that IV (R = CO2H) had an α-CO group could not be confirmed by preparation of the C-13 epimer but was proven by conclusive evidence obtained by electron-impact induced fission of I. I (25 mg.) was converted to the corresponding acetylene, 8α,13-oxidolabd-14-yne (XI) by the method used for preparation of VII and the product distilled gave 10 mg. sample, b0.1 130°, [α]D 7° (c 1.2). Similarly, 2.5 mg. III gave 8α,13-ioxidolabd-14-yne (XII), m. 99-102°. Examination of the cracking patterns of I and II showed a proportionally greater loss of a Me group from I, suggesting that the substituents on the oxide ring are in a more congested environment in I. Similar expts. were conducted with the acetylenic compds. XI and XII and indicated a preferential loss of a Me group in XI. It was concluded that in I, C-16 was in the more congested axial β-position. The cracking patterns were obtained conventionally with an ion accelerating voltage of 2 kv. with an electron beam energy of 50 e.v. The appearance potentials were obtained according to R. (loc. cit.).

IT 5468-59-7P, Pyran-2-malonic acid, tetrahydro-, diethyl ester
49574-99-4P, Pyran-2-malonic acid, tetrahydro-
RL: PREP (Preparation)
(preparation of)

RN 5468-59-7 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)



RN 49574-99-4 CAPLUS
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)



L6 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1956:69394 CAPLUS
DOCUMENT NUMBER: 50:69394
ORIGINAL REFERENCE NO.: 50:13001e-i,13002a-i,13003a-b
TITLE: Stereochemical studies of olefinic compounds. V. Further observations on the ring fission of 3-chlorotetrahydrofurans and -pyrans
AUTHOR(S): Crombie, L.; Gold, J.; Harper, S. H.; Stokes, B. J.
CORPORATE SOURCE: Imperial Coll. Sci. Technol., London
SOURCE: Journal of the Chemical Society (1956) 136-42
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:69394

AB cf. C.A. 50, 1595b. Dry Cl passed into 30 g. tetrahydropyran in 30 mL. CCl4 containing 0.2 g. iodine employing conditions described previously (C. and H., C.A. 45, 1009e) gave 34 g. trans-2,3-dichlorotetrahydropyran (I), b20 86-90°, nD20 1.4945, identical with the product (II) obtained by the addition of Cl to dihydropyran (C.A. 45, 1008f), b20 88-90°, nD20 1.4946. I and II had identical IR spectra (29 bands) in the region 700-3300 cm.-1 2,3-Dihydrofuran (III) (10 g., prepared by isomerization from 2,5-dihydrofuran) treated in 75 mL. dry Et2O and dry Cl until a faint green tint persisted, the green color discharged with a few drops of III, and the whole concentrated and distilled gave 16.1 g. trans-2,3-dichlorotetrahydrofuran (IV), b22 65-70°, nD20 1.4840, identical with the product (V) obtained by the chlorination of THF, b21 63-6°, nD20 1.4841; in the region 800-3300 cm.-1, IV and V had identical IR spectra. The procedure of C. and H. (loc. cit.) was used to prepare a series of 2-alkyl-3-chlorotetrahydrofurans; while each was fractionated through a 120 + 2.5 cm. glass helix-packed column, complete resolution of cis and trans isomers was not accomplished and data for the best fractions are given (alkyl group, % over-all yield, b.p. (trans), nD19, d19, b.p. (cis), nD19, d19): Me, 83, trans- (VI), 130°, 1.4424, 1.078, cis- (VII), 147°, 1.4532, 1.104; Et, 87, trans- (VIII), 150°, 1.4459, 1.046, cis- (IX), 165°, 1.4556, 1.075; iso-Pr, 57, trans- (X), 164°, 1.4482, 1.027, cis- (XI), 178°, 1.4568, 1.053. The Me3C isomers decomposed rapidly on distillation and fractionation was not possible. Assignment of configurations of these compds. was based on the Auwers-Skita rules as well as rate studies on their dehydrochlorination with EtONa in EtOH. Ring fission of the above stereoisomers with Na is summarized as follows (isomer, product, % yield, b.p., nD20): VI, α-MeCH:CHCH2CH2OH, 64, 136-7°, 1.4342; VII, β-MeCH:CHCH2CH2OH, 70, 137-8°, 1.4357; VIII, α-EtCH:CHCH2CH2OH, 59, 63-4° (16 mm.), 1.4383; IX, β-EtCH:CHCH2CH2OH, 84, 64-5° (16 mm.), 1.4393; X, α-Me2CHCH:CHCH2CH2OH (XII), 86, 71-3° (15 mm.), 1.4372; and XI, β-Me2CHCH:CHCH2CH2OH (XIII), 70, 70-4° (16 mm.), 1.4335. XII and XIII gave 1-naphthylurethanes, m. 56° and 63°, resp. (from petr. ether). The preparation of pure reference compds. is summarized as follows: stereospecific reduction of the corresponding acetylene with Na in liquid NH3 gave trans-MeCH:CHCH2CH2OH (XIV) and trans-EtCH:CHCH2CH2OH; cis-MeCH:CHCH2CH2OH was a carefully fractionated specimen obtained by the partial hydrogenation of MeC .tplbond.CCH2CH2OH over Pd-CaCO3 (contamination with XIV was very small, about 1-2%); cis-EtCH:CHCH2CH2OH was a carefully purified specimen isolated from Brazilian Mentha arvensis oil. In anal., use was made of the fact that the trans alcs. showed strong absorption at 967 cm.-1, almost nonexistent in the cis alcs., both

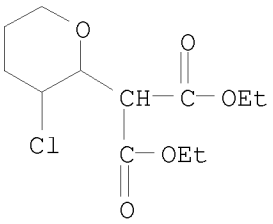
showed a strong band at 1040 cm.-1 due to the HO group, and the HO and trans band were of comparable intensity. The rates of reaction of the stereoisomeric 2-alkyl-3-chlorotetrahydrofuran (XV) with EtONa in EtOH were determined as follows: 4 identical ampuls containing 0.1 mol XV in 10 mL. absolute EtOH and 20 mL. of a solution prepared by dissolving 16 g. Na in absolute EtOH, then diluting to 500 mL. were sealed and immersed in a H2O bath at 100° for varying periods of time; subsequently, the ampul was broken in ice H2O and the liberated Cl- determined; the % reaction for each compound for 20, 54, 84 and 120 min. is summarized as follows: VI, 7.9, 21.0, 32.0, 45.3; VII, 16.0, 41.9, 57.0, 72.1; VIII, 8.9, 20.6, 32.6, 45.5; IX, 12.1, 32.0, 45.1, 58.5; X, 8.0, 21.1, 33.0, 46.0; and XI, 10.7, 29.1, 44.0; 57.0. To Me3CMgBr (from 300 g. Me3CBr and 55 g. Mg in Et2O) cooled in ice was added dropwise 210 g. 2,3-dichlorotetrahydrofuran to give 153 g. crude 2-tert-butyl-3-chlorotetrahydrofuran (XVI), b19 80-105°; attempted fractional distillation gave tars; rapid distillation gave 6 cuts, 2 (XVII and XVIII) of which b5 61-4°, and b5 75-80°, resp. As above, either XVII or XVIII 4.8 g. and 1.5 g. Na in 50 mL. Et2O gave 2.3 g. Me3CCH:CHCH2CH2OH, b16 80-1°, nD20 1.4470. trans-BuCH:CH(CH2)3OH (156 g.) gave 139 g. trans-BuCH:CH(CH2)3Br (XIX), b22 83-5°, nD20 1.4690. The Grignard reagent from 135 g. XIX, 16 g. Mg, and 150 mL. Et2O, and 0.5 mol 2,3-dichlorotetrahydropyran (XX) reacted in the usual manner to give 81 g. mixture of isomers of 2-chlorotetrahydro-2-(trans-4-nonenyl)pyran (XXI), b0.3 130-50°; as above, 80 g. XXI and 17 g. Na in 140 mL. Et2O gave 45.5 g. trans-trans-tetradeca-4,9-dien-1-ol (XXII), b5 139-41°, nD20 1.4590; XXII hydrogenated over Raney Ni gave myristyl alc. (XXIII), b15 165-8°, m. 38°, which gave myristic acid, b1 121-2°, m. 57°. The RMgX compound (1.2 mol) was treated with 1 mol XX in the usual manner and added via a glass bridge under N pressure in 4-5 h. to 2 g. atoms powdered Na under Et2O gave the alk-4-en-1-olderiv. The presence of excess RMgX apparently retards the Na fission and care must be exercised in initiating the reaction. XX (160 g.) in 350 mL. Et2O and 10 g. LiAlH4 in 400 mL. Et2O treated in the usual manner, were decomposed with wet Et2O and dilute H2SO4, the Et2O layer separated, dried and distilled gave 70 g. 3-chlorotetrahydropyran (XXIV), b13 52-4°, b. 140-3°, nD20 1.4626. In similar fashion, 2,3-dichlorotetrahydrofuran gave 67% 3-chlorotetrahydrofuran (XXV), b30 59-61°, nD20 1.4532. XXIV (8.5 g.) in 30 mL. Et2O added slowly to 4 g. Na in 15 mL. Et2O gave 4.4 g. CH2:CH(CH2)3OH, b. 134-7°, nD20 1.4301; 1-naphthylurethane, m. 62°. Similarly, XXV gave 79% CH2:CH(CH2)2OH, b. 111-14°, nD20 1.4218; 1-naphthylurethane, m. 77° (from petr. ether). XXIV (34.4 g.) added dropwise to NaNH2 [from 26 g. Na in 500 mL. liquid NH3 in the presence of Fe(NO3)3], 200 mL. Et2O added, the whole stirred overnight, concentrated aqueous NH3 added, the Et2O layer separated, the aqueous phase repeatedly extracted with Et2O, the combined Et2O exts. dried, concentrated and distilled gave 12.4 g. 3,4-dihydropyran (XXVI), b. 85-8°, nD20 1.4406, and 4.9 g. HC.tplbond.C(CH2)3OH, b. 150-5°, nD20 1.4488 (1-naphthylurethane, m. 83°). Similarly, 3-chlorotetrahydro-2-methylfuran gave 28% MeC.tplbond.C(CH2)2OH, b. 153-160° (1-naphthylurethane, m. 119°), and 32% 2,3-dihydro-5-methylfuran (XXVII), b. 78-85°; 3-chloro-2-ethyltetrahydrofuran gave 34% 5-ethyl-2,3-dihydrofuran, b. 100-10°, and 20% EtC.tplbond.C(CH2)2OH, b. 164-6° (1-naphthylurethane, m. 85°); and 3-chlorotetrahydro-2-isopropylfuran gave 37% 2,3-dihydro-5-isopropylfuran, b. 120-7° and 17% Me2CHC.tplbond.C(CH2)2OH, b. 160-3° (1-naphthylurethane, m. 88°). III, XXVI, or XXVII gave no acetylenic alcs. when treated with NaNH2 in liquid NH3. Freshly distilled 96% CH2:CHCHO (295 g.), 350 mL.

C6H6 and 4 g. quinol in a 1 l. stirred stainless steel autoclave heated rapidly to 160° and kept 4 h. at 160° gave 108 g. 2-formyl-3,4-dihydropyran (XXVIII), b17 52-3°, nD20 1.4646. XXVIII (149 g.) in 88 g. each of EtOH and C6H6 and 21 g. Raney Ni hydrogenated at 60° and 30 atmospheric gave 126 g. tetrahydro-2-hydroxymethylpyran (XXIX), b. 180-3°, nD20 1.4566. Adding (19 g.) SOCl2 to 58 g. XXIX in 44 g. C5H5N, keeping the temperature below 25°, stirring 3 h., extracting with 7 + 30 mL. portions of Et2O, washing the Et2O exts. with H2O, drying, concentrating and distilling gave di(tetrahydro-2-pyranylmethyl) sulfite, b0.07 135-7°, nD20 1.4833. 2-Chloromethylpyran (16.8 g.) and 6 g. Na as above gave 10.8 g. CH2:CH(CH2)4OH; 1-naphthylurethane, m. 62°. 2,3-Dichlorotetrahydropyran (31 g.) added to NaCH(CO3Et)2 [from 5.95 g. Na 150 mL. absolute EtOH, and 41.5 g. CH2(CO2Et)2], the mixture refluxed 0.5 h., concentrated partially in vacuo, H2O added to the residue, the whole extracted with Et2O, the Et2O exts. concentrated and distilled repeatedly gave 3.0 g. 3-chloro-2-(diethoxycarbonylmethyl)tetrahydropyran, b0.08 110-15°, nD15 1.4642.

IT 857176-45-5P, Pyran-2-malonic acid, 3-chlorotetrahydro-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 857176-45-5 CAPLUS

CN Propanedioic acid, 2-(3-chlorotetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)



L6 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

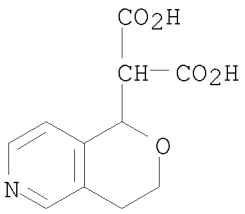
ACCESSION NUMBER: 1956:16374 CAPLUS
DOCUMENT NUMBER: 50:16374
ORIGINAL REFERENCE NO.: 50:3432i,3433a-f
TITLE: Synthesis of 5-(2-hydroxyethyl)quinuclidine-2-carboxylic acid
AUTHOR(S): Rubtsov, M. V.; Yakhontov, L. N.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Sci. Research Chem.-Pharm. Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1955), 25, 1183-9
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 48, 7610a; preceding abstract Heating 20 g. 3-(2-acetoxyethyl)-4-methylpyridine, 21.3 g. di-Et dihydroxymalonate [prepared by oxidation of CH2(CO2Et)2 with SeO2 followed by treatment of the di-Et mesoxalic ester with calculated amount of H2O], and 65 ml. Ac2O 10 hrs. on a steam bath gave 19.7 g. mixed 3-(2-acetoxyethyl)-4-(2,2-dicarbethoxyvinyl)pyridine (I) and II [R = CH(CO2Et)2] (IIa), b0.2 180-200°. The mixture in Et2O was treated dropwise with alc. HCl and the oil which separated was rubbed with Et2O, yielding 11% IIa.HCl, m. 147-8°; further addition of alc. HCl to the solution gave 36.1% I.HCl, m. 111-12°; I picrate, m.

115-16°. Refluxing I.HCl with 8% alc. HCl 8 hrs. gave 99.2% IIa.HCl. Heating 0.5 g. IIa.HCl salt with 50 ml. 17% HCl at reflux 8 hrs., treating with C and evaporating in vacuo, followed by rubbing the residue with absolute EtOH gave 97.6% II (R = CH2CO2H).HCl, decompose 200.5-1.5°; treatment with NaOAc gave the free acid, decompose 192-4°, identical with that formed by hydrolysis of 3-(2-acetoxyethyl)-4-(3,3,3-trichloro-2-hydroxypropyl)pyridine (cf. preceding abstract). Hydrogenation of I.HCl in dry EtOH over PtO2 at room temperature gave 3-(2-acetoxyethyl)-4-(2,2-dicarbethoxyethyl)pyridine-HCl, m. 109-10° (from EtOH-Et2O); continued hydrogenation for 15 days gave 3-(2-acetoxyethyl)4-(2,2-dicarbethoxyethyl)piperidine-HCl (III), oil; free base, b0.3 194-7° (some decomposition), nD20 1.4790; HCl salt, picrate, picrolonate, and reineckate were oils. III (11.3 g.) in CHCl3 was treated with 4.76 g. Br at room temperature over 9 hrs., the solvent removed and the residue treated with aqueous K2CO3 (25%), yielding oily 3-(2-acetoxyethyl)-4-(2,2-dicarbethoxy-2-bromoethyl)piperidine, which refluxed with pyridine 2 hrs. gave after treatment with K2CO3 45.2% 5-(2-acetoxyethyl)-2,2-dicarbethoxyquinuclidine, b0.5 110-70°, nD20 1.4809, d20 1.133, mixture of 2 stereoisomers; all salts were oils. Refluxing 16 hrs. with concentrated HCl gave 89.2% 5-(2-hydroxyethyl)quinuclidine-2-carboxylic acid-HCl, amorphous powder; treatment with NaOH and evaporation gave the free acid, the same being obtained by treatment of the HCl salt with Ag2O, followed by decomposition of the Ag salt with H2S. The free acid is a very hygroscopic powder. Treatment with ale. HCl at reflux 12 hrs., followed by base gave 10.2% Et 5-(2-hydroxyethyl)quinuclidine-2-carboxylate, b0.26 102-15°; HCl salt, picrate and methiodide were oils. Absorption spectra of I, II, and compds. related to II (loc. cit.) are shown graphically.

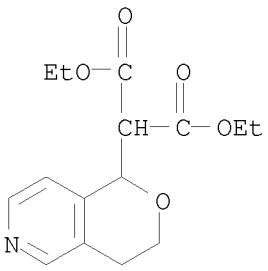
IT 857177-75-4P, 1H-Pyrano[4,3-c]pyridine-1-malonic acid, 3,4-dihydro-, hydrochloride 857177-82-3P, 1H-Pyrano[4,3-c]pyridine-1-malonic acid, 3,4-dihydro-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 857177-75-4 CAPLUS
CN Propanedioic acid, 2-(3,4-dihydro-1H-pyrano[4,3-c]pyridin-1-yl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 857177-82-3 CAPLUS
CN Propanedioic acid, 2-(3,4-dihydro-1H-pyrano[4,3-c]pyridin-1-yl)-, 1,3-diethyl ester (CA INDEX NAME)



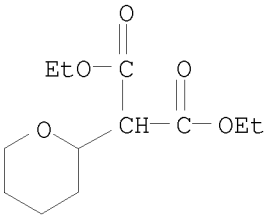
L6 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:892 CAPLUS
DOCUMENT NUMBER: 48:892
ORIGINAL REFERENCE NO.: 48:168g-i,169a-d
TITLE: Preparation of l-2-aminomethyltetrahydropyran
AUTHOR(S): Zelinski, Robert P.; Peterson, Norman G.; Wallner, Hope R.
CORPORATE SOURCE: De Paul Univ., Chicago
SOURCE: Journal of the American Chemical Society (1952), 74, 1504-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:892

AB The method of Schudel and Rice (C.A. 45, 6223i) yielded 78% Et dl-2-tetrahydropyranylmalonate (I), b1-2 120-2°, n20D 1.4480, d20 1.075. I (29.7 g.) and 366 cc. 2N HCl boiled 2 hrs. and fractionated yielded dl-tetrahydro-2-pyranylacetic acid (II), b2 110-12°, m. 55-7°. I (48.8 g.) and 40.0 g. NaOH in 300 cc. 33% EtOH boiled 1.5 hrs., 0.059 mole 4N HCl added, the solution concentrated to 150 cc., 0.39 mole 4N HCl added, the solution extracted 5 hrs. continuously with Et2O and the Et2O evaporated yielded 36.8 g. dl-2-tetrahydropyranylmalonic acid (III), m. 140-1° (decomposition). III (36.8 g.) heated at 140-50° and the residue distilled in vacuo yielded 21.6 g. II, m. 52-3°. II (10 g.) and 25 cc. SOCl2 heated 1 hr. on the steam bath yielded 8.4 g. acid chloride (IV), b3 60-5°. IV (0.88 g.), 3 cc. PhNH2, and 25 cc. C6H6 warmed 3 min. on the steam bath yielded 0.58 g. anilide, m. 83-4°. IV (2.3 g.) in 60 cc. petr. ether (ice bath) treated with NH3 yielded 83% amide (V), m. 99-101°. IV and NH4OH yielded 81%. V (14 g.) added to 193 cc. ice cold water containing 24 g. Br and 23 g. NaOH, the mixture held 3 hrs. at 0°, heated to 90°, diluted with 300 cc. water, distilled into 100 cc. 3N HCl, 300 cc. water added and distillation resumed, the acid solution evaporated almost to dryness, the residue treated with 8 g. NaOH in 200 cc. water and the solution extracted 8 hrs. with C6H6 yielded 5.5 g. dl-2-aminoethyltetrahydropyran (VI), b. 167-9°, n20D 1.4589, d20 0.987; N-benzoyl derivative, m. 116-18°. VI (0.59 g.) and 1.0 g. III treated with 10 cc. 10% KOH yielded N-(2-tetrahydropyranylacetyl)-2-aminomethyltetrahydropyran, m. 67-9°. VI (8.0 g.) in 10 cc. hot MeOH added to 10.5 g. d-tartaric acid in 25 cc. MeOH, the mixture filtered hot, and let stand 2 days at 5° yielded 14 g. d-VI salt (VII), m. 160-1°, [α]27D 40.3° (c 1.35, water). VII (3.7 g.) with 20 cc. 10% NaOH extracted 6 hrs. with C6H6 yielded 0.8 g. d-VI (VIII), b. 167-9°, [α]24D 8.3° (homogeneous). The N-benzoyl derivative (VIIIA) of VIII m. 112-13°, [α]24D 28.3° (c 2.9, CHCl3). Quinine (52.6 g.) in 450 cc. hot C6H6 and 23.3 g. II in 15

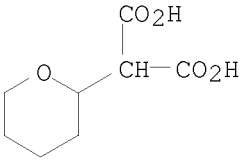
cc. hot C6H6 mixed and filtered, and let stand 2 days at 5° yielded 10.1 g. quinine salt (IX) of l-II, m. 162-3°, [α]27D -136.3° (c 0.7, EtOH). IX (10.0 g.) in 50 cc. CHCl3 shaken with 60 cc. 2N NaOH, the aqueous phase extracted 4 hrs. with CHCl3, neutralized with 1.5N HCl, extracted 6 hrs. with fresh CHCl3 and the CHCl3 solution distilled yielded 3.4 g. l-II (X), b4 120-5°, m. 37-8°, [α]27D -5.67° (c 15, EtOH). D-Deoxyephedrine was less satisfactory for resolution. X (3.0 g.) by the preceding reactions yielded 2.0 g. d-V (XI), m. 84-5°, [α]24D 12.5° (c 1.6, EtOH). XI (2.0 g.) yielded 1.0 g. VIII, b. 167-9°, [α]24D 6.40°; VIIIA m. 111-13°, [α]25D 25.4° (c 1.75, CHCl3).

IT 5468-59-7P, Pyran-2-malonic acid, tetrahydro-, diethyl ester
49574-99-4P, Pyran-2-malonic acid, tetrahydro-, dl-
RL: PREP (Preparation)
(preparation of)

RN 5468-59-7 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)



RN 49574-99-4 CAPLUS
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)



L6 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1951:36243 CAPLUS
DOCUMENT NUMBER: 45:36243
ORIGINAL REFERENCE NO.: 45:6223h-i,6224a
TITLE: Tetrahydropyranylmalonic esters
INVENTOR(S): Schudel, John G.; Rice, Robb V.
PATENT ASSIGNEE(S): Gane's Chemical Works, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2522966		19500919	US 1948-24673	19480501 <--

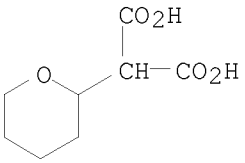
GI For diagram(s), see printed CA Issue.
AB Di-Et α-ethyltetrahydropyran-2-malonate (I), an intermediate for

barbiturate syntheses, is prepared from NaCEt(CO2Et)2 (II) and 2-chlorotetrahydropyran (III). Thus, a solution of III (prepared by saturating toluene (IV) 200 cc. containing tetrahydropyran 88 g. with HCl gas at -10 to 0°) is added at 20-30° to a suspension of II in IV (prepared from HCEt(CO2Et)2 188 and NaH 25 g. in 200 cc. IV at 90°), held 3 hrs., stirred with H2O 350 ml., separated, and fractionated in vacuo to give I, O.(CH2)4.CHCEt(CO2Et)2, b2 115-17°, n20D 1.4525. Similarly were prepared the following compds. O.(CH2)4.CHCR(CO2Et)2, R given: H, b7 135-40°, n20D 1.4463; Ph, m. 78-81.5°, b7 169-71°, n25D 1.5021; PrMeCH, b5 132-5°, n20D 1.4583; iso-Pr, b6 126-30° n20D 1.4570; Bu, b3 121-5°, n20D 1.4535; iso-Bu, b6 123-4°, n20D 1.4541; iso-Am, b5 125°, n20D 1.4530; C6H13, b3 158-9°, n20D 1.4540; CH2:CHCH2, b10 151-4°, n20D 1.4611; Δ2,3-cyclopentyl, b4 142-6°, n20D 1.4790; cyclohexyl, b2 149-54°, n20D 1.4760; CH2:CMeCH2, b1.5 117-20°, n20D 1.4642; CH2:CBrCH2, b5 155-7°, n20D 1.4860; PhCH2, m. 80-1°.

IT 49574-99-4, Pyran-2-malonic acid, tetrahydro- (derivs.)

RN 49574-99-4 CAPLUS

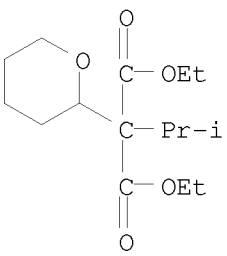
CN Propanedioic acid, (tetrahydro-2H-pyran-2-yl)- (9CI) (CA INDEX NAME)



IT 857173-23-0P, Pyran-2-malonic acid, tetrahydro-α-isopropyl-, diethyl ester 857173-30-9P, Pyran-2-malonic acid, tetrahydro-α-isopentyl-, diethyl ester 857173-37-6P, Pyran-2-malonic acid, tetrahydro-α-isobutyl-, diethyl ester 857176-30-8P, Pyran-2-malonic acid, α-hexyltetrahydro-, diethyl ester 857176-37-5P, Pyran-2-malonic acid, α-ethyltetrahydro-, diethyl ester 857176-53-5P, Pyran-2-malonic acid, α-butyltetrahydro-, diethyl ester 857176-62-6P, Pyran-2-malonic acid, α-2-bromoallyltetrahydro-, diethyl ester 857176-70-6P, Pyran-2-malonic acid, α-benzyltetrahydro-, diethyl ester 857176-77-3P, Pyran-2-malonic acid, α-allyltetrahydro-, diethyl ester 857226-25-6P, Pyran-2-malonic acid, tetrahydro-α-2-methylallyl-, diethyl ester 857226-33-6P, Pyran-2-malonic acid, tetrahydro-α-1-methylbutyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 857173-23-0 CAPLUS

CN Propanedioic acid, 2-(1-methylethyl)-2-(tetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)



RN 857173-30-9 CAPLUS
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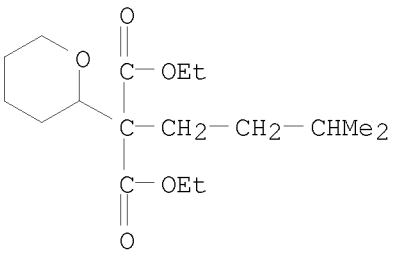
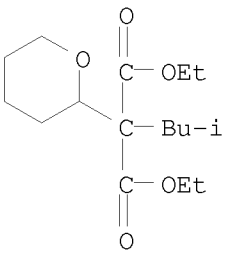


RN 857173-37-6 CAPLUS
CN Propanedioic acid, 2-(2-methylpropyl)-2-(tetrahydro-2H-pyran-2-yl)-, 1,3-diethyl ester (CA INDEX NAME)



RN 857176-30-8 CAPLUS
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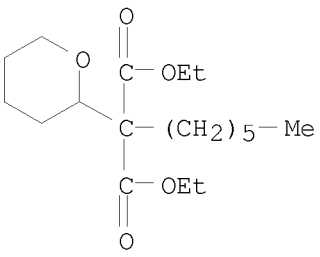

RN 857176-37-5 CAPLUS
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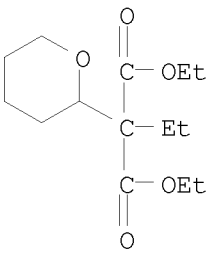

RN 857176-53-5 CAPLUS
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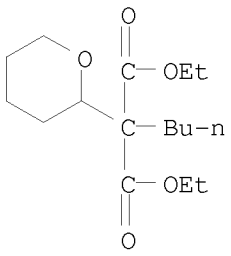

RN 857176-62-6 CAPLUS
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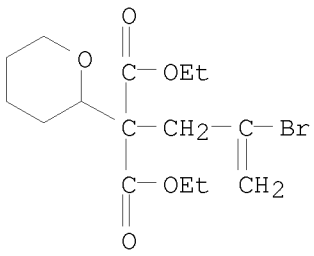

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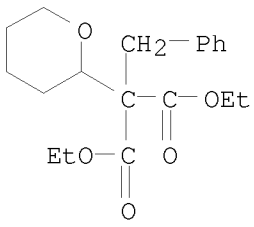

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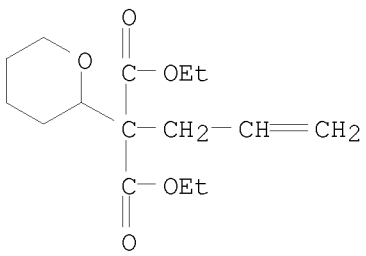

RN 857226-25-6 CAPLUS
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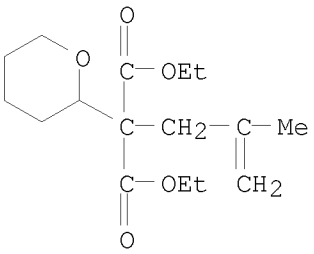

RN 857226-33-6 CAPLUS
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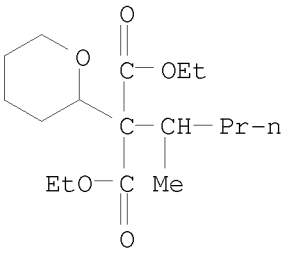

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE	-48.00	-48.00

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DICTIONARY FILE UPDATES: 28 APR 2008 HIGHEST RN 1017984-01-8

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experimental property data in the original document. For information
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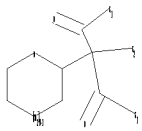

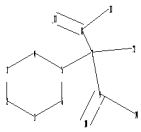

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G1:O,N

G2:C,H,Cl,Br,F

Match level :
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L7   STRUCTURE UPLOADED

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L7 HAS NO ANSWERS
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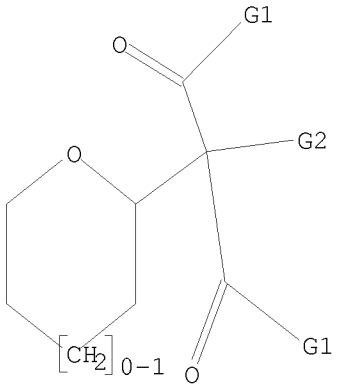

G1 O,N

G2 C,H,Cl,Br,F

Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
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PROJECTED ANSWERS:              11 TO      389

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SEARCH TIME: 00.00.01

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FULL ESTIMATED COST                                  178.36     693.12

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    0.00     -48.00

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FILE COVERS 1907 - 29 Apr 2008 VOL 148 ISS 18
FILE LAST UPDATED: 28 Apr 2008 (20080428/ED)

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http://www.cas.org/infopolicy.html

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L10         89 L9

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L4          133 S L1 FULL

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L7              STRUCTURE UPLOADED
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L9          155 S L7 FULL

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L12  ANSWER 1 OF 53  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2005:497502  CAPLUS
DOCUMENT NUMBER:         143:53440
TITLE:                   Substituted benzoimidazole compounds as transcription
                         factor-modulating compounds useful as anti-infectives
INVENTOR(S):             Levy, Stuart B.; Alekshun, Michael N.; Podlogar, Brent
                         L.; Ohemeng, Kwasi; Verma, Atul K.; Warchol, Tadeusz;
                         Bhatia, Beena; Bowser, Todd; Grier, Mark
```

PATENT ASSIGNEE(S): Paratek Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 463 pp., Cont.-in-part of U.S. Ser. No. 139,591.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 20050124678	A1	20050609	US 2003-700661	20031103	
CA 2445515	A1	20021104	CA 2002-2445515	20020506	<--
AU 2002367953	A1	20040106	AU 2002-367953	20020506	
EP 1524974	A2	20050427	EP 2002-807554	20020506	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2005519998	T	20050707	JP 2004-515557	20020506	
US 20030229065	A1	20031211	US 2002-139591	20020814	<--
US 20040106553	A1	20040603	US 2003-602562	20030624	

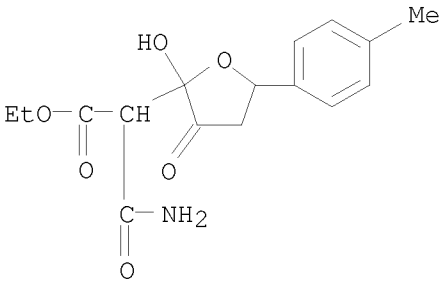
PRIORITY APPLN. INFO.:		
US 2001-288660P	P	20010504
US 2002-139591	A2	20020814
US 2002-423319P	P	20021101
US 2002-425916P	P	20021113
WO 2002-US14255	W	20020506
US 2002-391345P	P	20020624
US 2002-421218P	P	20021025
US 2002-429142P	P	20021126
US 2003-458935P	P	20030331

OTHER SOURCE(S): MARPAT 143:53440

AB Substituted benzoimidazole compds. useful as anti-infectives that decrease resistance, virulence, or growth of microbes are provided. Methods of making and using substituted benzoimidazole compds., as well as pharmaceutical prepns. thereof, in, e.g., reducing antibiotic resistance and inhibiting biofilms. The present invention identifies microbial transcription factors, especially transcription factors of the AraC-XylS family, as virulence factors in microbes and shows that inhibition of these factors reduces the virulence of microbial cells. Because these transcription factors control virulence, rather than essential cellular processes, the development of resistance is much less likely.

IT 634189-30-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(substituted benzoimidazole compds. as transcription factor-modulating compds. useful as anti-infectives)

RN 634189-30-3 CAPLUS
CN 2-Furanacetic acid, α-(aminocarbonyl)tetrahydro-2-hydroxy-5-(4-methylphenyl)-3-oxo-, ethyl ester (CA INDEX NAME)



L12 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:971725 CAPLUS
DOCUMENT NUMBER: 140:35893
TITLE: Transcription factor modulating compounds and methods of use thereof
INVENTOR(S): Levy, Stuart B.; Alekshun, Michael N.; Podlogar, Brent L.; Ohemeng, Kwasi; Verma, Atul K.; Warchol, Tadeusz; Bhatia, Beena
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 301 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030229065	A1	20031211	US 2002-139591	20020814 <--
CA 2445515	A1	20021104	CA 2002-2445515	20020506 <--
WO 2004001058	A2	20031231	WO 2002-US14255	20020506 <--
WO 2004001058	A3	20050303		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002367953	A1	20040106	AU 2002-367953	20020506
EP 1524974	A2	20050427	EP 2002-807554	20020506
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2005519998	T	20050707	JP 2004-515557	20020506
US 20050124678	A1	20050609	US 2003-700661	20031103

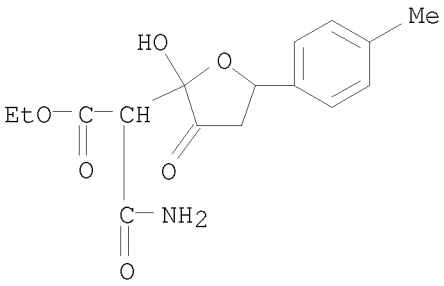
PRIORITY APPLN. INFO.:	US 2001-288660P	P	20010504
	WO 2002-US14255	W	20020506
	US 2002-139591	A2	20020814
	US 2002-423319P	P	20021101
	US 2002-425916P	P	20021113

OTHER SOURCE(S): MARPAT 140:35893
AB Methods for identifying compound useful as anti-infectives that decrease resistance, virulence, or growth of microbes are provided. In one embodiment, the method comprises contacting a microbial cell comprising:

(1) a selectable marker under the control of a transcription factor responsive element and (2) a transcription factor, with a compound under conditions which allow interaction of the compound with the microbial cell; and measuring the ability of the compound to affect the growth or survival of the microbial cell as an indication of whether the test compound modulates the activity of a transcription factor.

IT 634189-30-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(transcription factor modulating compds. as anti-infectives agents that decrease resistance and virulence and growth identified by determining marker under control of responsive element)

RN 634189-30-3 CAPLUS
CN 2-Furanacetic acid, α-(aminocarbonyl)tetrahydro-2-hydroxy-5-(4-methylphenyl)-3-oxo-, ethyl ester (CA INDEX NAME)



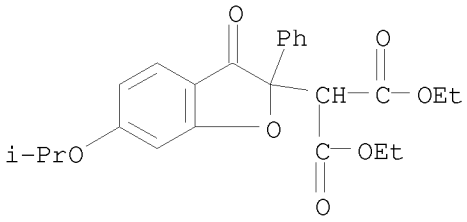
L12 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:612860 CAPLUS
DOCUMENT NUMBER: 138:24605
TITLE: Studies on synthesis of 3(2H)-benzofuranone derivatives
AUTHOR(S): Bokotey, Sandor; Kovari-Radkai, Maria; Podanyi, Benjamin; Ritz, Imola; Hanusz, Miklos; Batori, Sandor
CORPORATE SOURCE: CHINOIN Pharmaceutical and Chemical Works Co. Ltd., Budapest, H-1325, Hung.
SOURCE: Synthetic Communications (2002), 32(15), 2325-2343
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24605

AB Two known methods were used for synthesis of 2,6-disubstituted-3(2H)-benzofuranone derivs. It was found that depending on the reaction conditions, degradation products or the products of oxidation were isolated. This latter reaction became the main process when the ring closure was performed starting from methoxybenzoin or 2-propoxy-desoxybenzoin and di-Et bromomalonate or chloromalonate to give D,L- and meso-dimers of the substituted 3(2H)-benzofuranones. Among the products prepared in this study were 6,6'-dihydroxy-2,2'-dimethyl-[2,2'-bibenzofuran]-3,3'(2H,2'H)-dione (dimer), 2-phenyl-3,6-benzofurandiol, 6-hydroxy-2-phenyl-3(2H)-benzofuranone.

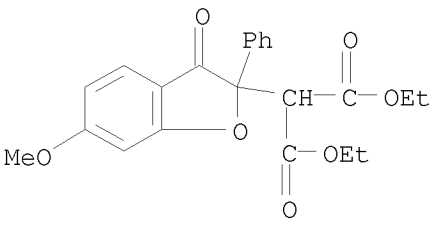
IT 478068-90-5, 1-(2,4-Dimethoxyphenyl)-2-phenylethanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and reactions of 3(2H)-benzofuranone derivs.)

RN 478068-90-5 CAPLUS

CN Propanedioic acid, [2,3-dihydro-6-(1-methylethoxy)-3-oxo-2-phenyl-2-benzofuranyl]-, diethyl ester (9CI) (CA INDEX NAME)



IT 478068-83-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of 3(2H)-benzofuranone derivs.)
RN 478068-83-6 CAPLUS
CN Propanedioic acid, (2,3-dihydro-6-methoxy-3-oxo-2-phenyl-2-benzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

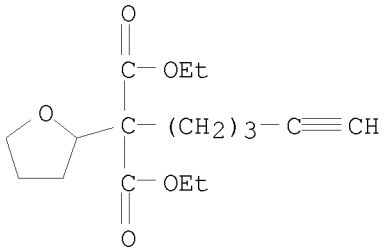
L12 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:689145 CAPLUS
DOCUMENT NUMBER: 136:53539
TITLE: Lithium malonate enolates as precursors for radical reactions - convenient induction of radical cyclizations with either radical or cationic termination
AUTHOR(S): Jahn, Ullrich; Hartmann, Philip; Dix, Ina; Jones, Peter G.
CORPORATE SOURCE: Institut fur Organische Chemie, Technische Universitat Braunschweig, Braunschweig, 38106, Germany
SOURCE: European Journal of Organic Chemistry (2001), (17), 3333-3355
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:53539
AB Lithium malonate enolates are oxidized to their radicals by ferrocenium hexafluorophosphate (I) uCl2. Trapping by TEMPO to produce the piperidinyloxymalonates, dimerization to tetracarboxylates, or radical 5-exo cyclizations are possible subsequent reaction steps following radical generation. The structure of the radical cyclization acceptor dets. the outcome of the overall reaction sequence. Tertiary benzylic, alkyl, and α-alkoxy radicals are oxidized by I. The carbenium ions are stabilized by nucleophilic trapping or deprotonation to give oxabicyclooctanes and cyclopentanedicarboxylates. Secondary alkyl and

vinyl radicals are not oxidized and, in the absence of trapping reagents, form radical-derived products. Radical 5-exo cyclization of alkenylmalonates induced by CuCl2 was also efficient. At least for alkyl radicals, however, ligand transfer is the exclusive stabilization pathway, giving access to chloroalkylcyclopentane derivs.. Radical scavenging studies revealed that malonyl radical trapping is slow, so that 5-exo cyclizations occurred. The cyclized radicals couple with TEMPO to afford oxygenated cyclopentane derivs., depending on the rate of radical SET oxidation The reaction behavior of some of the products was investigated. Mechanistic issues are discussed and implications for synthetic planning are given.

IT 381733-76-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and radical cyclization of malonate enolates)

RN 381733-76-2 CAPLUS

CN Propanedioic acid, 4-pentynyl(tetrahydro-2-furanyl)-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:227167 CAPLUS

DOCUMENT NUMBER: 128:294480

TITLE: Ring-chain tautomerism in 2-(2,2-dicyano-1-methylethenyl)benzoic acid and related compounds

AUTHOR(S): Kolsaker, Per; Arukwe, Joe; Barcoczy, Jozsef; Wiberg, Are; Fagerli, Anne Kristine

CORPORATE SOURCE: Department of Chemistry, University of Oslo, Oslo, N-0315, Norway

SOURCE: Acta Chemica Scandinavica (1998), 52(4), 490-498
CODEN: ACHSE7; ISSN: 0904-213X

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

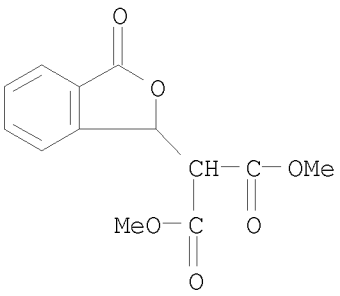
AB Ring chain tautomerism with slow interconversion (compared with the NMR timescale) was observed in solns. of 2-(2,2-dicyano-1-methylethenyl)benzoic acid (3e), obtained by Knoevenagel condensation of 2-acetylbenzoic acid with malononitrile, forming the ring tautomer 3-dicyanomethyl-3-methylphthalide (4e) in admixt. with 3e. Similar condensations of 2-formylbenzoic acid with Me cyanoacetate or malononitrile give 2-(2-cyano-2-methoxycarbonylethenyl)benzoic acid (3b) and 2-(2,2-dicyanoethenyl)benzoic acid (3d), resp., which in solution also exhibit the same tautomerism to give the ring tautomers, 3-(cyanomethoxycarbonylmethyl)phthalide (4b) and 3-(dicyanomethyl)phthalide (4d), resp. Condensation of 2-formylbenzoic acid with di-Me malonate gave only the ring compound, 3-(dimethoxycarbonylmethyl)phthalide (4a). Attempts to synthesize

2-(2-cyano-2-methoxycarbonyl-1-methylethenyl)benzoic acid (3c) by methylation of the tri-Me silyl ester of 3b with diazomethane led to the ring form of 3c, viz. 3-cyanomethoxycarbonylmethyl-3-methylphthalide (4c) as an equimolar mixture of two diastereomers. No tautomerism was observed when the benzene ring was replaced by a thiophene ring (7a, 7b and 8) or an aliphatic double bond (9). Solid state spectra (IR and NMR) indicated that all compds. carrying two cyano groups at the double bond, except the aliphatic compound 9, were in the open-chain form, while all the others were in the ring form. Equilibrium studies for compound (3e.dblharw.4e) indicated increased stability for the chain form 4e with increasing solvent polarity, Determination of the free energy change, ΔG°, and of the free energy of activation, $\Delta G^{\ddagger}$, for the tautomerization in deuteriochloroform (using 1H NMR spectroscopy) indicated that, in this solvent, a concerted process from the starting material 3e to the anion of 4e is taking place. It is also postulated that a similar reaction path is followed in the other solvents used in this investigation, all belonging to the solvent class 'protophobic dipolar aprotic solvents'.

IT 206202-35-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring-chain tautomerism in 2-(2,2-dicyano-1-methylethenyl)benzoic acid and related compds.)

RN 206202-35-9 CAPLUS

CN Propanedioic acid, (1,3-dihydro-3-oxo-1-isobenzofuranyl)-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:296330 CAPLUS

DOCUMENT NUMBER: 122:187920

TITLE: An efficient glycosylation reaction of 1-hydroxy sugars with various nucleophiles using a catalytic amount of activator and hexamethyldisiloxane

AUTHOR(S): Mukaiyama, Teruaki; Matsubara, Koki; Hora, Miyuki

CORPORATE SOURCE: Fac. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SOURCE: Synthesis (1994), (Spec. Issue), 1368-73
CODEN: SYNTBF; ISSN: 0039-7881

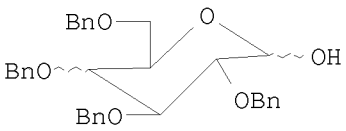
PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:187920

GI



I

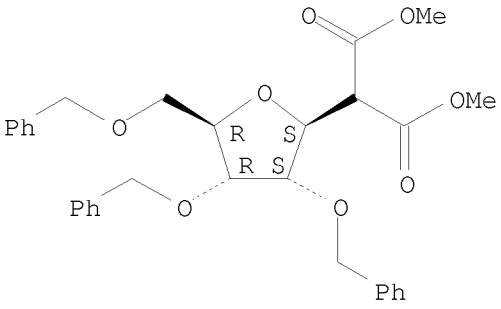
AB In the presence of hexamethyldisiloxane and anhydrous calcium sulfate, a catalytic amount of activator such as tin(II) trifluoromethanesulfonate, ytterbium trifluoromethanesulfonate, lanthanum trifluoromethanesulfonate or tin(II) chloride smoothly promotes the glycosidation reactions between 1-hydroxy sugars, e.g. I, and free alcs., amino acids, electron-rich aromatic compds. or silylated nucleophiles to produce various O-, C- or N-glycosides stereoselectively in high yields. In the case of oxygen or nitrogen nucleophiles, β-ribosides are formed, except that α-ribosides are obtained predominantly in the presence of lithium perchlorate. In the case of carbon nucleophiles such as electron-rich aromatic compds. or silyl enol ethers derived from carbonyl compds., perfect β-selectivity is shown either in the presence or absence of lithium perchlorate. Further, pyranosyl substrates such as glucose or galactose afford the corresponding α-anomers, except with electron-rich aromatic compds.

IT 96689-88-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(tin and lanthanum triflates-catalyzed stereoselective glycosidation of alcs.)

RN 96689-88-2 CAPLUS

CN Propanedioic acid, [2,3,5-tris-O-(phenylmethyl)-β-D-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L12 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:427740 CAPLUS

DOCUMENT NUMBER: 119:27740

TITLE: Synthesis of 1-substituted 12-oxahexacyclo[7.2.1.02,8.03,7.04,11.06,10]dodecanes and their transformation into pentacyclo[6.3.0.02,6.03,10.05,9]undecane derivatives

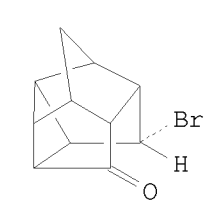
AUTHOR(S): Aleksandrov, Alexander M.; Kashyap, Ram P.; Pehk, Tynis J.; Petrenko, Alexander E.; Watson, William H.

CORPORATE SOURCE: Inst. Bioorg. Chem., Kiev, 252094, Ukraine

SOURCE: Journal of Organic Chemistry (1993), 58(7), 1831-4
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:27740
GI



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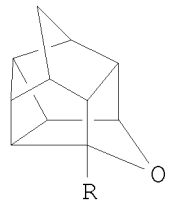
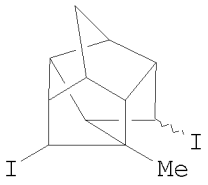
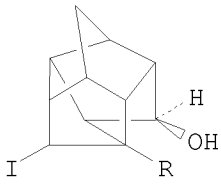


II



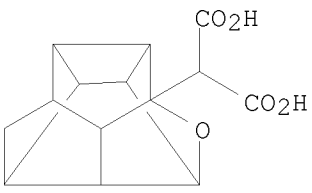
III



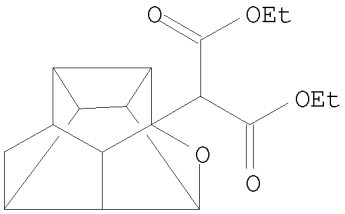
IV

AB The reaction of nucleophilic reagents (organomagnesium and organosodium compds. containing active methylene groups) with exo-11-bromopentacyclo[5.4.0.02,6.03,10.05,9]undecan-8-one (I) leads to the formation of 1-substituted-12-oxahexacyclo[7.2.1.02,8.03,7.04,11.06,10]dodecanes [II; R = Me, Ph, PhCH2, CH(CO2Et)2, CH(CN)CO2Et] which can be used in the synthesis of trishomocubane dervis. It is shown, using the 1-methyl- and 1-phenyl-substituted 12-oxadodecanes II (R = Me, Ph), that iodotrimethylsilane readily cleaves the ether bond at C(1). The resulting carbonium ions rearrange to form 1,7,11-trisubstituted pentacyclo[6.3.0.02,6.03,10.05,9]undecanes III and IV (R = Me, Ph). The crystal structures of alc. III and IV (R = Ph) were determined

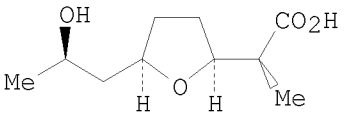
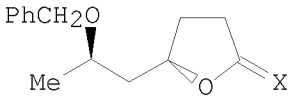
IT 147661-31-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)
RN 147661-31-2 CAPLUS
CN Propanedioic acid, (octahydro-2,6,3,5-ethanediylidene-2H-pentaleno[1,6-bc]furan-2-yl)- (9CI) (CA INDEX NAME)



IT 147661-21-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)
RN 147661-21-0 CAPLUS
CN Propanedioic acid, (octahydro-2,6,3,5-ethanediylidene-2H-pentaleno[1,6-bc]furan-2-yl)-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:426149 CAPLUS
DOCUMENT NUMBER: 117:26149
ORIGINAL REFERENCE NO.: 117:4707a,4710a
TITLE: A synthesis of (+)-nonactic acid by means of the sulfur-ylide rearrangement
AUTHOR(S): Honda, Toshio; Ishige, Hirohide; Araki, Junko; Akimoto, Saeko; Hirayama, Kazuo; Tsubuki, Masayoshi
CORPORATE SOURCE: Inst. Med. Chem., Hoshi Univ., Tokyo, 142, Japan
SOURCE: Tetrahedron (1992), 48(1), 79-88
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:26149
GI

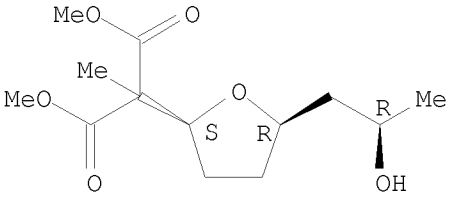

I

II

AB (+)-Nonactic acid (I) has been synthesized by employing a condensation of tetrahydro-2-furanthione II (X = S) with N2C(CO2Me)2 in the presence of Rh(OAc)2 as a key reaction to give II [X = C(CO2Me)2] which was reduced stereoselectively over Pd in HCl-MeOH.

IT 139932-13-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 139932-13-1 CAPLUS
CN Propanedioic acid, methyl[tetrahydro-5-(2-hydroxypropyl)-2-furanyl]-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

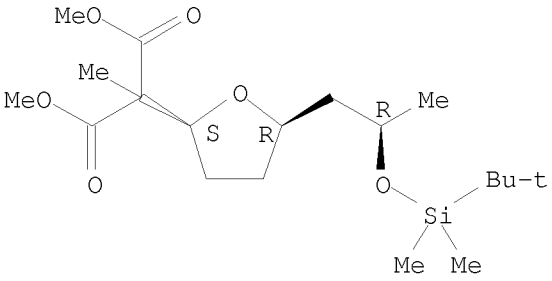
Absolute stereochemistry.



IT 139932-12-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

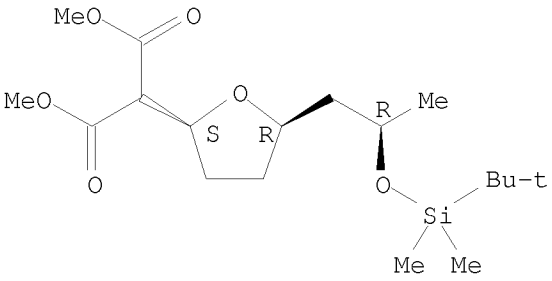
(Reactant or reagent)
(preparation and desilylation of)
RN 139932-12-0 CAPLUS
CN Propanedioic acid, [5-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]tetrahydro-2-furanyl]methyl-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



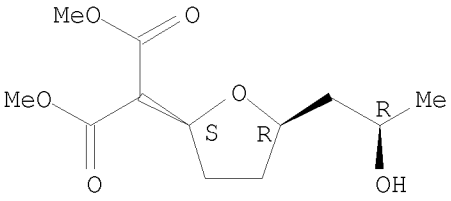
IT 139932-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 139932-11-9 CAPLUS
CN Propanedioic acid, [5-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]tetrahydro-2-furanyl]-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



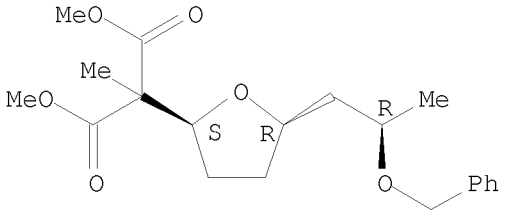
IT 139932-10-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation of)
RN 139932-10-8 CAPLUS
CN Propanedioic acid, [tetrahydro-5-(2-hydroxypropyl)-2-furanyl]-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



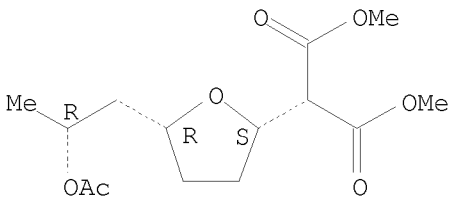
IT 139932-09-5P 139932-16-4P 140146-25-4P
140146-26-5P 140146-27-6P 140146-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 139932-09-5 CAPLUS
CN Propanedioic acid, methyl[tetrahydro-5-[2-(phenylmethoxy)propyl]-2-furanyl]-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



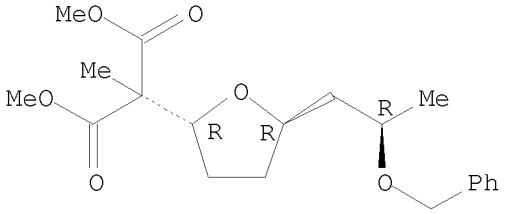
RN 139932-16-4 CAPLUS
CN Propanedioic acid, [5-[2-(acetyloxy)propyl]tetrahydro-2-furanyl]-, dimethyl ester, [2S-[2α,5α(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



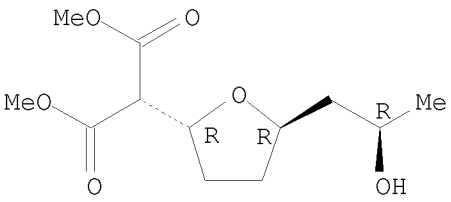
RN 140146-25-4 CAPLUS
CN Propanedioic acid, methyl[tetrahydro-5-[2-(phenylmethoxy)propyl]-2-furanyl]-, dimethyl ester, [2R-[2α,5β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



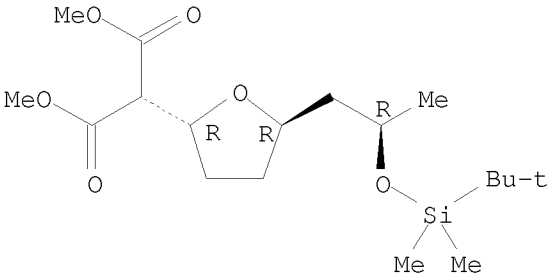
RN 140146-26-5 CAPLUS
CN Propanedioic acid, [tetrahydro-5-(2-hydroxypropyl)-2-furanyl]-, dimethyl ester, [2R-[2α,5β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



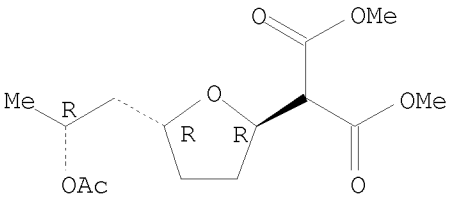
RN 140146-27-6 CAPLUS
CN Propanedioic acid, [5-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]tetrahydro-2-furanyl]-, dimethyl ester, [2R-[2α,5β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 140146-28-7 CAPLUS
CN Propanedioic acid, [5-[2-(acetyloxy)propyl]tetrahydro-2-furanyl]-, dimethyl ester, [2R-[2α,5β(R*)]]- (9CI) (CA INDEX NAME)

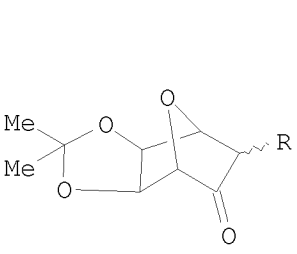
Absolute stereochemistry.



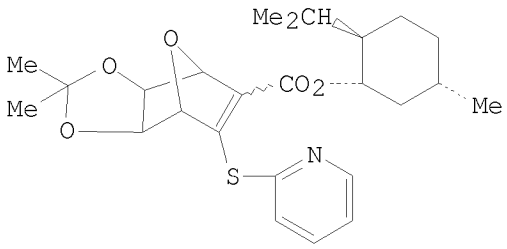
L12 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:559532 CAPLUS
DOCUMENT NUMBER: 115:159532
ORIGINAL REFERENCE NO.: 115:27331a,27334a
TITLE: New approach to sugar derivatives by Pummerer reactions of optically active sulfoxide and sulfide having a 7-oxabicyclo[2.2.1]heptane ring system
AUTHOR(S): Takahashi, Tamiko; Kotsubo, Hironori; Koizumi, Toru
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (7), 1667-71
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:159532

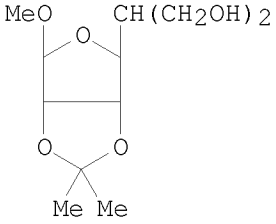
GI



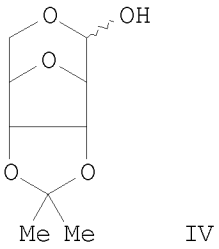
I



II



III



IV

AB Pummerer reactions of 3-(2-pyridylsulfinyl)-2-oxabicyclo[2.2.1]heptane-2-carboxylate and the corresponding sulfide, which were obtained by an asym. Diels-Alder reaction of the (S)s-3-(2-pyridylsulfinyl)acrylate, gave the β-keto ester I (R = menthyloxycarbonyl) and the vinyl sulfide II in 62 and 87% yield, resp. I (R = menthyloxycarbonyl) was transformed into the C(5)-branched-chain sugar derivative III by successive Baeyer-Villiger oxidation and stereoselective cleavage of the resulting lactone. Dealkoxycarbonylation of I (R = menthyloxycarbonyl) afforded I (R = H). In addition, upon ozonolysis, II was converted into the D-2,5-anhydroallose derivative IV.

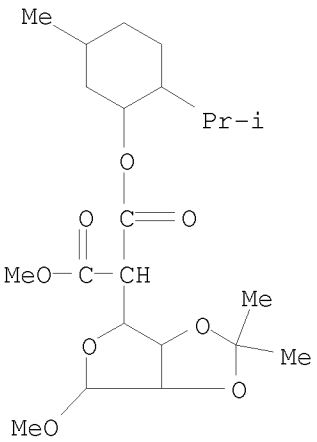
IT 136340-72-2P 136378-65-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

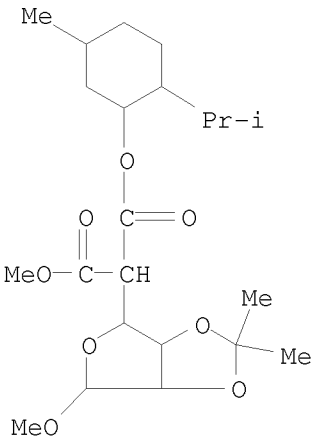
(preparation and reduction of)

RN 136340-72-2 CAPLUS

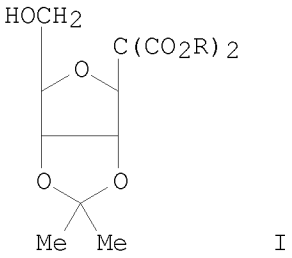
CN β-L-Allofuranosiduronic acid, methyl 5-deoxy-5-(methoxycarbonyl)-2,3-O-(1-methylethylidene)-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, [1R-(1α,2β,5α)]- (9CI) (CA INDEX NAME)



RN 136378-65-9 CAPLUS
CN β-L-Allofuranosiduronic acid, methyl 5-deoxy-2,3-O-(1-methylethylidene)-5-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]carbonyl]-, methyl ester, [1R-(1α,2β,5α)]- (9CI) (CA INDEX NAME)



L12 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:193211 CAPLUS
DOCUMENT NUMBER: 110:193211
ORIGINAL REFERENCE NO.: 110:32093a,32096a
TITLE: High-pressure-mediated Diels-Alder reaction of di-L-menthyl acetoxymethylenemalonate with furan: enantioselective synthesis of β-D-ribofuranosylmalonate, a prospective synthon for C-nucleoside
AUTHOR(S): Katagiri, Nobuya; Akatsuka, Hidenori; Kaneko, Chikara; Sera, Akira
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Tetrahedron Letters (1988), 29(42), 5397-400
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:193211
GI



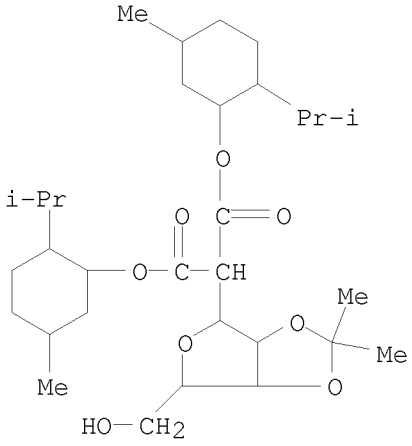
I

AB β-D-Ribofuranosylmalonate (D)-I was synthesized via high-pressure Diels-Alder reaction of furan with di-l-menthyl acetoxymethylenemalonate, followed by reductive retrograde aldol C-C bond fission. A mechanism accounting for the observed diastereoselectivity in the Diels-Alder reaction is proposed.
IT 120315-73-3P 120408-71-1P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective synthesis of)

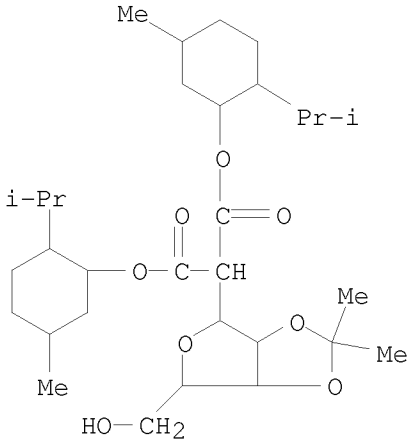
RN 120315-73-3 CAPLUS

CN Propanedioic acid, [2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, bis[5-methyl-2-(1-methylethyl)cyclohexyl] ester, [1R-[1α(1R*,2S*,5R*),2β,5α]]- (9CI) (CA INDEX NAME)



RN 120408-71-1 CAPLUS

CN Propanedioic acid, [2,3-O-(1-methylethylidene)-β-L-ribofuranosyl]-, bis[5-methyl-2-(1-methylethyl)cyclohexyl] ester, [1R-[1α(1R*,2S*,5R*),2β,5α]]- (9CI) (CA INDEX NAME)

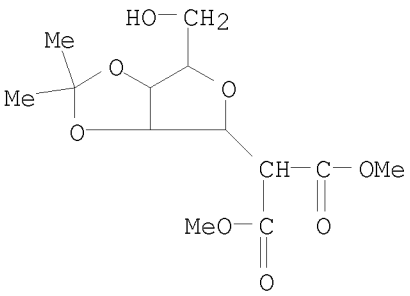


IT 117269-44-0P 117269-45-1P

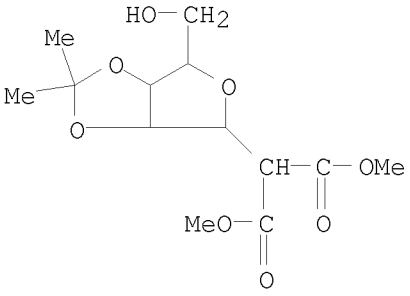
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 117269-44-0 CAPLUS

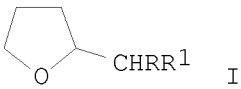
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-β-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



RN 117269-45-1 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-α-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:32739 CAPLUS
DOCUMENT NUMBER: 106:32739
ORIGINAL REFERENCE NO.: 106:5483a,5486a
TITLE: Synthesis of tetrahydrofurans from active methylene compounds via radical cyclization
AUTHOR(S): Moriya, Osamu; Urata, Yoshikiyo; Ikeda, Yoshikazu; Ueno, Yoshio; Endo, Takeshi
CORPORATE SOURCE: Dep. Chem., Natl. Def. Acad., Yokosuka, 239, Japan
SOURCE: Journal of Organic Chemistry (1986), 51(24), 4708-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:32739
GI



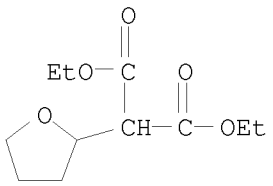
I

AB Tetrahydrofurans I (R = CN, CO2Et, R1 = CO2Et; R = Ac, R1 = CO2Me, Bz) were prepared by treating HC[O(CH2)3Cl]3 with active methylenes RCH2R1 and subjecting the resulting RR1C:CHO(CH2)3Cl to radical cyclization by treatment with Bu3SnH in the presence of AIBN.
IT 70398-41-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from active methylene compound via radical cyclization)

RN 70398-41-3 CAPLUS

CN Propanedioic acid, 2-(tetrahydro-2-furanyl)-, 1,3-diethyl ester (CA INDEX NAME)



L12 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:541726 CAPLUS

DOCUMENT NUMBER: 103:141726

ORIGINAL REFERENCE NO.: 103:22687a,22690a

TITLE: Oxonium ion electrophiles: synthesis of the hypotensive oudenone

AUTHOR(S): Bates, Hans Aaron; Farina, James

CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA

SOURCE: Journal of Organic Chemistry (1985), 50(20), 3843-5

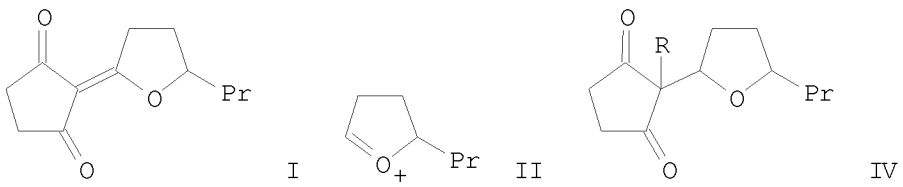
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:141726

GI



AB The hypotensive oudenone (I), from the culture filtrate of Oudenasiella radicata was synthesized via oxonium ion II. Acid-catalyzed C-alkylation of 1,3-cyclopentanedione (III) with 5-propyltetrahydro-2-furanol gave dihydrooudenone [IV, R = H(V)]. In contrast, alkylation of III with 2-chloro-5-propyltetrahydrofuran was unsuccessful. Unsatn. was introduced into V by treatment with N-(phenylthio)succinimide to give IV (R = SPh) followed by oxidation to the corresponding sulfoxide and elimination of phenylsulfenic acid to give I.

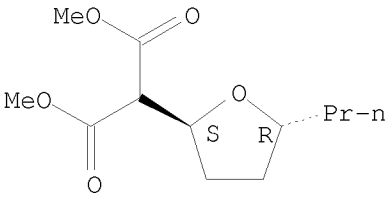
IT 97974-57-7P 97974-58-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 97974-57-7 CAPLUS

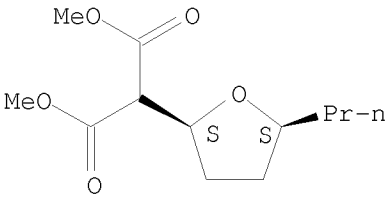
CN Propanedioic acid, (tetrahydro-5-propyl-2-furanyl)-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

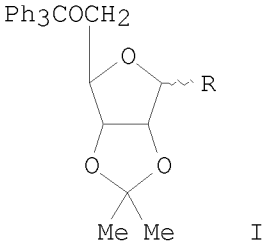


RN 97974-58-8 CAPLUS
CN Propanedioic acid, (tetrahydro-5-propyl-2-furanyl)-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



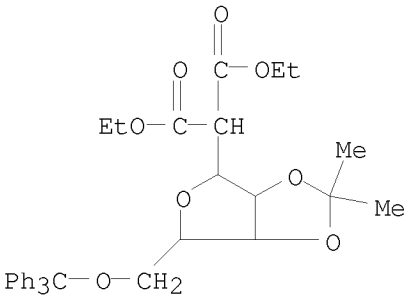
L12 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:471122 CAPLUS
DOCUMENT NUMBER: 99:71122
ORIGINAL REFERENCE NO.: 99:11059a,11062a
TITLE: Synthetic C-nucleosides. Synthesis of C-glycoside precursors of C-nucleosides through activation of the anomeric hydroxyl group
AUTHOR(S): Germain, F.; Chapleur, Y.; Castro, B.
CORPORATE SOURCE: Lab. Chim. Org. II, CNRS, Nancy, 54037, Fr.
SOURCE: Tetrahedron (1982), 38(24), 3593-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



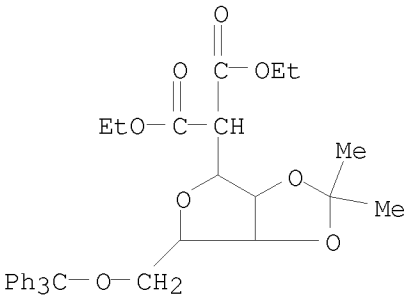
I

AB Treatment of ribose derivative I [R = β-OP+(NMe2)3 Cl-] (II) with Na+ C-HR1R2 (R1 = CN, R2 = CN, CO2Me, CONH2; R1 = R2 = CO2Et) in THF or DMF at ambient temperature gave I (R = CHR1R2, R1 and R2 as before), predominantly or exclusively as the α-anomers. E.g., II with 5 equiv Na+ C-H(CN)2 in THF (added at -40°, allowed to rise to ambient temperature) gave, after hydrolysis, I [R = α-CH(CN)2] in 41% yield.

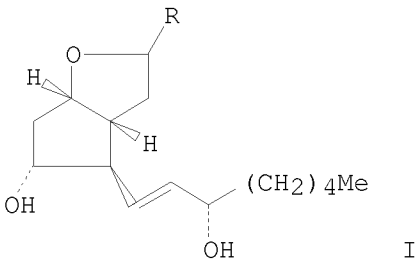
IT 56781-37-4P 56781-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56781-37-4 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 56781-38-5 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:405393 CAPLUS
DOCUMENT NUMBER: 99:5393
ORIGINAL REFERENCE NO.: 99:977a,980a
TITLE: Synthesis of prostacyclin analogs via Knoevenagel condensation
AUTHOR(S): Ivanics, J.; Simonidesz, V.; Galambos, G.; Kormoczy, P.; Kovacs, G.
CORPORATE SOURCE: Chinoin Pharm. Chem. Works Ltd., Budapest, H-1325, Hung.
SOURCE: Tetrahedron Letters (1983), 24(3), 315-18
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

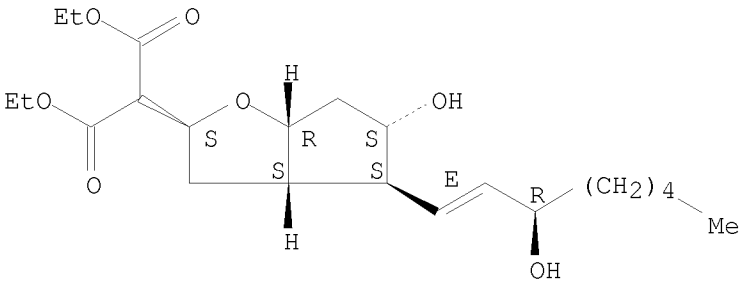
AB Prostacyclin precursors were readily prepared in 76-92% yield by Knoevenagel condensation of hemiacetal I (R = OH) (II) with activated methylene compds. E.g., reaction of II with (MeCO)2CH2 without solvent in the presence of piperidine at room temperature gave I [R = CH(COMe)2] in 80% yield. I [R = CHR1CO(CH2)2CO2Et; R1 = CO2Et, SO2C6H4Me-p], prepared analogously, gave 4-oxo-PGI1 [I; R = CH2CO(CH2)2CO2Et] on hydrolysis and reductive cleavage-hydrolysis, resp.

IT 85993-86-8P 85993-97-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 85993-86-8 CAPLUS

CN Propanedioic acid, [hexahydro-5-hydroxy-4-(3-hydroxy-1-octenyl)-2H-cyclopenta[b]furan-2-yl]-, diethyl ester, [2α,3aα,4α(1E,3S*),5β,6aα]- (9CI) (CA INDEX NAME)

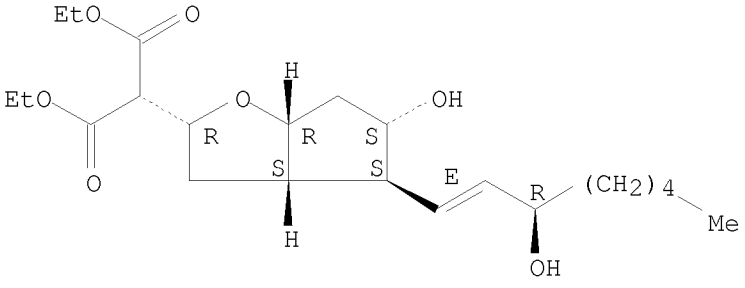
Relative stereochemistry.
Double bond geometry as shown.



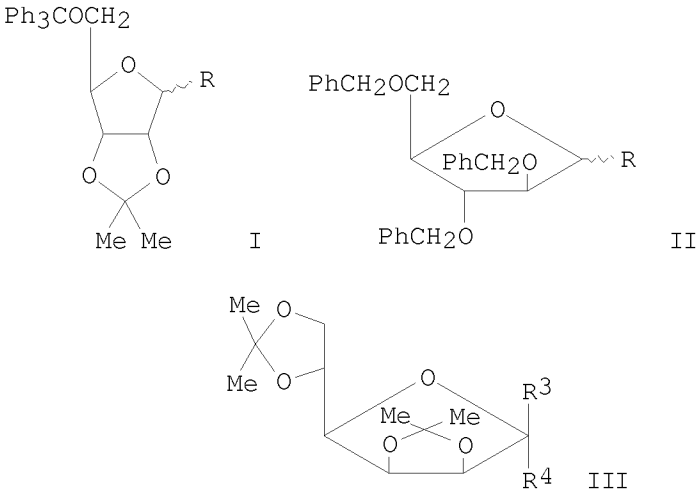
RN 85993-97-1 CAPLUS

CN Propanedioic acid, [hexahydro-5-hydroxy-4-(3-hydroxy-1-octenyl)-2H-cyclopenta[b]furan-2-yl]-, diethyl ester, [2α,3aβ,4β(1E,3R*),5α,6aβ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L12 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:198634 CAPLUS
DOCUMENT NUMBER: 98:198634
ORIGINAL REFERENCE NO.: 98:30219a,30222a
TITLE: A convenient synthesis of C-glycofuranosylmalonates and related derivatives
AUTHOR(S): Germain, Francoise; Chapleur, Yves; Castro, Bertrand
CORPORATE SOURCE: Lab. Chim. Org., Univ. Nancy, Vandoeuvre les Nancy, F-54 506, Fr.
SOURCE: Synthesis (1983), (2), 119-21
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

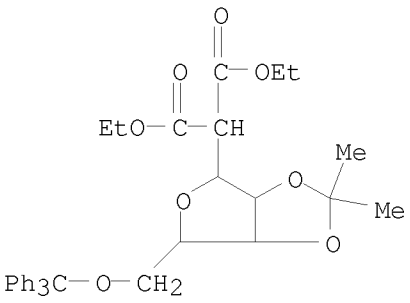


AB Reaction of ribose (I; R = OH) with NaCHR1R2 (R1 = cyano, R2 = cyano, CONH2, CO2Me; R1 = R2 = CO2Et) in THF at room temperature gave 30-84% I (R = CHR1R2). In the case of I [R = CH(CN)2] only the α-anomer was formed, whereas in other cases a mixture of α and β anomers was obtained. Analogously prepared was 82% α- and β-II [R = CH(CN)2] from II (R = OH), and 78% III [R3 = CH(CN)2, R4 = H] from III (R3 = H, R4 = OH). Phase transfer catalysis was also used in the preparation of I (R = CHR1R2; R1 = cyano, R2 = cyano, CONH2, CO2Me).

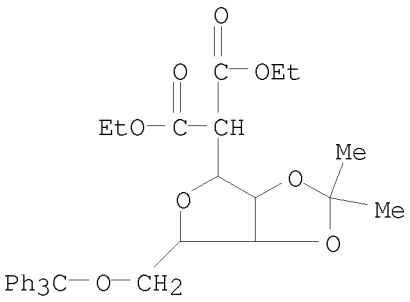
IT 56781-37-4P 56781-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 56781-37-4 CAPLUS

CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 56781-38-5 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



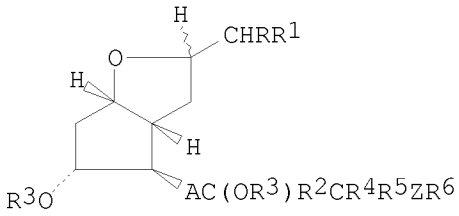
L12 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:179082 CAPLUS
DOCUMENT NUMBER: 98:179082
ORIGINAL REFERENCE NO.: 98:27211a,27214a
TITLE: 5-Substituted 4-oxo-PGI1 derivatives and their pharmaceutical compositions
INVENTOR(S): Simonidesz, Vilmos; Ivanics, Jozsef; Galambos, Geza; Papp, Agnes; Kovacs, Gabor; Skopal, Judit; Szilagyi, Ildiko
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt. , Hung.
SOURCE: Eur. Pat. Appl., 40 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 63323	A1	19821027	EP 1982-103025	19820408 <--
EP 63323	B1	19851030		
R: BE, CH, DE, FR, GB, IT, NL, SE				
HU 26764	A2	19830928	HU 1981-965	19810414 <--
HU 184948	B	19841128		
AT 8201390	A	19860215	AT 1982-1390	19820408 <--
AT 381303	B	19860925		
DK 8201656	A	19821015	DK 1982-1656	19820413 <--
FI 8201283	A	19821015	FI 1982-1283	19820413 <--

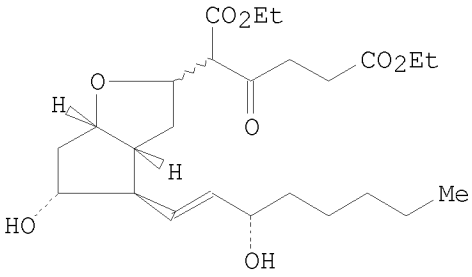
SU 1189335	A3	19851030	SU 1982-3425451		19820413 <--
IL 65490	A	19851129	IL 1982-65490		19820413 <--
JP 57183779	A	19821112	JP 1982-61194		19820414 <--
DD 202156	A5	19830831	DD 1982-238985		19820414 <--
CS 228922	B2	19840514	CS 1982-2661		19820414 <--
PL 129640	B1	19840531	PL 1982-235964		19820414 <--
US 4520018	A	19850528	US 1982-369543		19820419 <--
PRIORITY APPLN. INFO.:			HU 1981-965	A	19810414

OTHER SOURCE(S): MARPAT 98:179082

GI



I



II

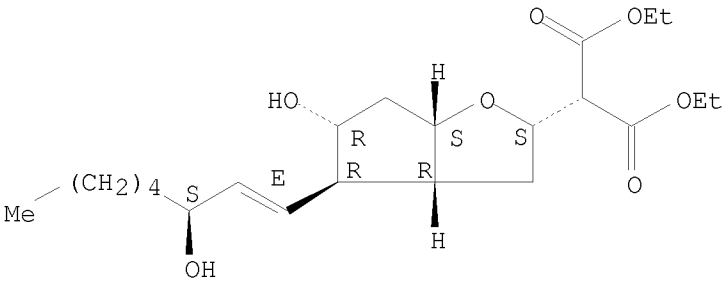
AB I (R = CO2H or derivative, NO2, arylthio, arylsulfonyl, etc.; A = trans-CH:CH, CH2CH2, C.tplbond.C; Z = CH2, O, NH; R1-6 = groups associated with prostaglandins) were prepared Thus, 3α,β-hydroxy-6β-(3S-hydroxy-1E-octenyl)-7α-hydroxy-2-oxabicyclo[3.3.0]octane was alkylated with di-Et 3-oxoadipate to give II, or, e.g., with O2N(CH2)4CO2Me to give 5-nitro-PGI1 Me ester.

IT 85492-92-8P 85550-86-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 85492-92-8 CAPLUS

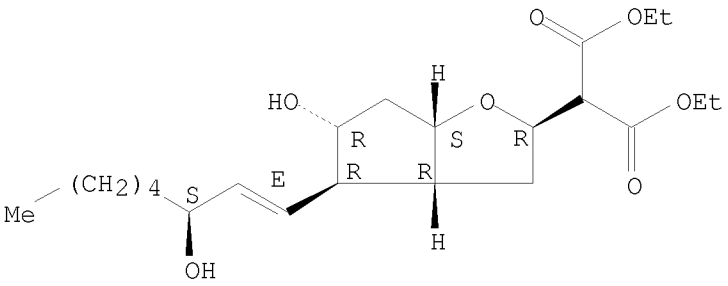
CN Propanedioic acid, [hexahydro-5-hydroxy-4-(3-hydroxy-1-octenyl)-2H-cyclopenta[b]furan-2-yl]-, diethyl ester, [2S-[2α,3aβ,4β(1E,3R*),5α,6aβ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 85550-86-3 CAPLUS
CN Propanedioic acid, [hexahydro-5-hydroxy-4-(3-hydroxy-1-octenyl)-2H-cyclopenta[b]furan-2-yl]-, diethyl ester, [2R-[2α,3aα,4α(1E,3S*),5β,6aα]]- (9CI) (CA INDEX NAME)

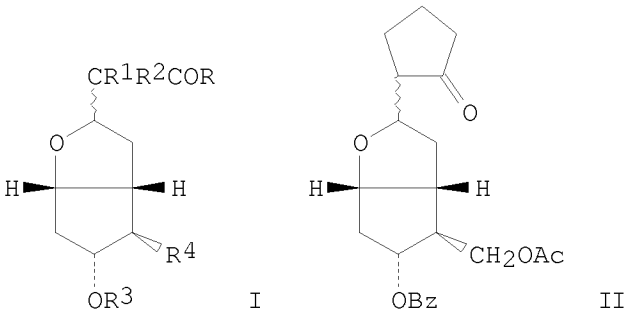
Absolute stereochemistry.
Double bond geometry as shown.

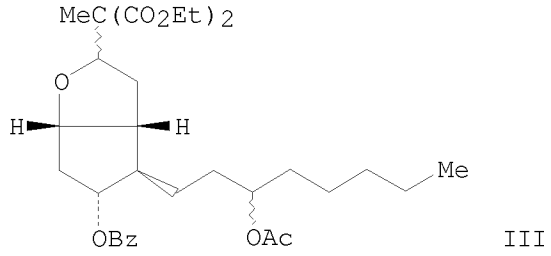


L12 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:89050 CAPLUS
DOCUMENT NUMBER: 98:89050
ORIGINAL REFERENCE NO.: 98:13579a,13582a
TITLE: 2-Oxa-bicyclo[3.3.0]octane derivatives and compositions containing them
INVENTOR(S): Vollenberg, Werner; Boehlke, Horst
PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 56 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 59307	A1	19820908	EP 1982-100317		19820118	<--
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE						
US 4430497	A	19840207	US 1982-349678		19820217	<--
HU 27168	A2	19831028	HU 1982-552		19820224	<--
DK 8200823	A	19820827	DK 1982-823		19820225	<--
JP 57156480	A	19820927	JP 1982-28248		19820225	<--
PRIORITY APPLN. INFO.:			DE 1981-3107248	A	19810226	

OTHER SOURCE(S): MARPAT 98:89050
GI



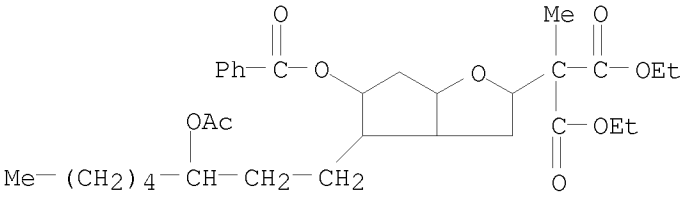


AB I, R-R4 were groups associated with prostaglandins, were prepared by conventional treatment (NaBH4 reduction, acetylation, silylation, etc.) of known compds. Typical of the .apprx.20 compds. prepared were II and III.

IT 84555-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as prostaglandin intermediate)

RN 84555-94-2 CAPLUS

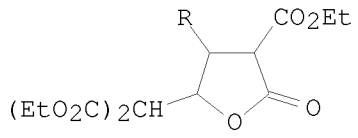
CN Propanedioic acid, [4-[3-(acetyloxy)octyl]-5-(benzoyloxy)hexahydro-2H-cyclopenta[b]furan-2-yl]methyl-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:22063 CAPLUS
DOCUMENT NUMBER: 92:22063
ORIGINAL REFERENCE NO.: 92:3749a,3752a
TITLE: Derivatives of γ-butyrolactones
INVENTOR(S): Avetisyan, A. A.; Boyadzhan, Zh. G.; Dangyan, M. T.
PATENT ASSIGNEE(S): Erevan State University, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1979, (25), 107.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
SU 672200	A1	19790705	SU 1976-2334380		19760315 <--
PRIORITY APPLN. INFO.:			SU 1976-2334380	A	19760315

GI



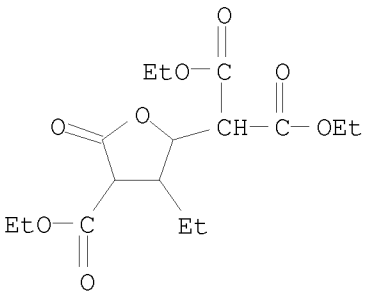
I

AB γ-Butyrolactones I (R = Et, iso-Pr, pentyl) were prepared by cyclocondensing CH2(CO2Et)2 with RCHBrCHO in aqueous medium at 35-40° in the presence of K2CO3.

IT 71674-96-9P 71674-97-0P 71674-98-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

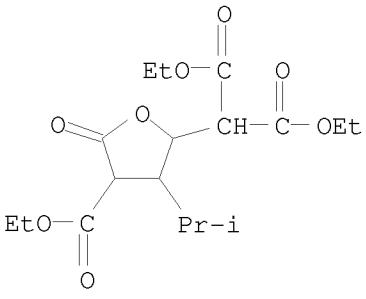
RN 71674-96-9 CAPLUS

CN Propanedioic acid, [4-(ethoxycarbonyl)-3-ethyltetrahydro-5-oxo-2-furanyl]-, diethyl ester (9CI) (CA INDEX NAME)



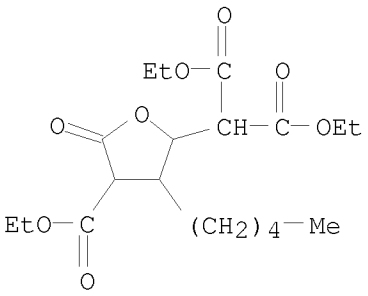
RN 71674-97-0 CAPLUS

CN Propanedioic acid, [4-(ethoxycarbonyl)tetrahydro-3-(1-methylethyl)-5-oxo-2-furanyl]-, diethyl ester (9CI) (CA INDEX NAME)

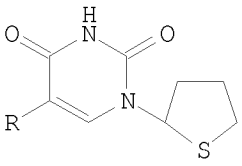


RN 71674-98-1 CAPLUS

CN Propanedioic acid, [4-(ethoxycarbonyl)tetrahydro-5-oxo-3-pentyl-2-furanyl]-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:491428 CAPLUS
DOCUMENT NUMBER: 91:91428
ORIGINAL REFERENCE NO.: 91:14767a,14770a
TITLE: Reactions of 2-chlorotetrahydrofuran and 2-chlorotetrahydrothiophene with phosphorus, carbon, and nitrogen nucleophiles
AUTHOR(S): Kruse, C. G.; Poels, E. K.; Van der Gen, A.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Leiden, Leiden, 2300 RA, Neth.
SOURCE: Journal of Organic Chemistry (1979), 44(16), 2911-15
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 91:91428
GI

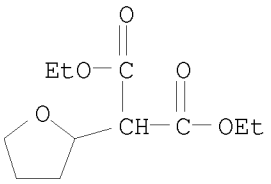


II

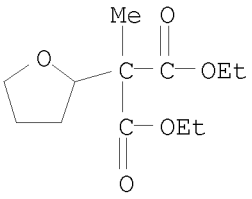
AB Reaction of 2-chlorotetrahydrofuran and 2-chlorotetrahydrothiophene (I) with P and C nucleophiles provided a number of synthetically useful THF and tetrahydrothiophene derivs. Reaction of I with N nucleophiles of low basicity likewise afforded the 2-substituted tetrahydrothiophenes. Preparation of N1-(tetrahydro-2-thienyl)uracil derivs. II (R = H, F) necessitated prior conversion of the uracil substrates into their bis-O-(trimethylsilyl) derivs.

IT 70398-41-3P 70398-42-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

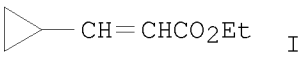
RN 70398-41-3 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2-furanyl)-, 1,3-diethyl ester (CA INDEX NAME)



RN 70398-42-4 CAPLUS
CN Propanedioic acid, methyl(tetrahydro-2-furanyl)-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:490767 CAPLUS
DOCUMENT NUMBER: 91:90767
ORIGINAL REFERENCE NO.: 91:14659a,14662a
TITLE: Decarbethoxylation and ring-opening reactions of 2-tetrahydrofuranyl-, 2-tetrahydrothienyl-, and 2-(1,3-dithianyl)-substituted esters
AUTHOR(S): Kruse, C. G.; Janse, A. C. V.; Dert, V.; Van der Gen, A.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Leiden, Leiden, 2300 RA, Neth.
SOURCE: Journal of Organic Chemistry (1979), 44(16), 2916-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

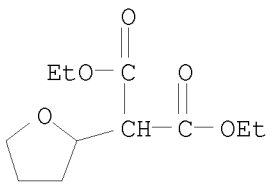


I

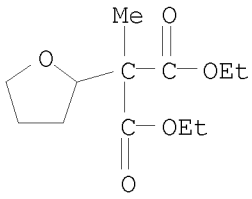
AB The course of decarbethoxylation of 2-tetrahydrofuranyl-, 2-tetrahydrothienyl- and 2-(1,3-dithianyl)-substituted malonic esters with NaCl/H2O in Me2SO is dependent on the nature of the substituents at the α-C atom. In several instances, selective decarbethoxylation provides monoesters; in other cases, stereoselective ring-opening reactions occur, leading to mixts. of α,β- and β,γ-unsatd. esters. In the absence of H2O, the cyclopropyl-substituted ester I is formed. Anions obtained by deprotonation of mono- and diesters undergo similar ring-opening reactions.

IT 70398-41-3 70398-42-4 70576-34-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(decarbethoxylation of)

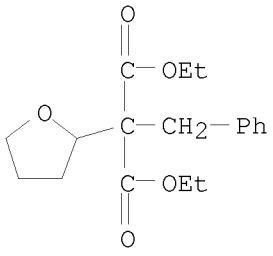
RN 70398-41-3 CAPLUS
CN Propanedioic acid, 2-(tetrahydro-2-furanyl)-, 1,3-diethyl ester (CA INDEX NAME)



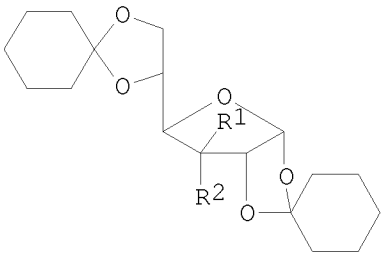
RN 70398-42-4 CAPLUS
CN Propanedioic acid, methyl(tetrahydro-2-furanyl)-, diethyl ester (9CI) (CA INDEX NAME)



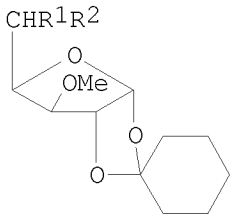
RN 70576-34-0 CAPLUS
CN Propanedioic acid, (phenylmethyl)(tetrahydro-2-furanyl)-, diethyl ester (9CI) (CA INDEX NAME)



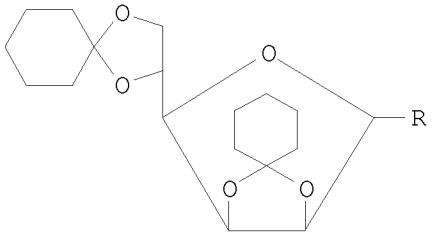
L12 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:170407 CAPLUS
DOCUMENT NUMBER: 88:170407
ORIGINAL REFERENCE NO.: 88:26875a,26878a
TITLE: C-Glycosyl malonates
AUTHOR(S): Zhdanov, Yu. A.; Alekseev, Yu. E.; Doroshenko, S. S.
CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR
SOURCE: Doklady Akademii Nauk SSSR (1978), 238(4), 868-9 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I



II



III

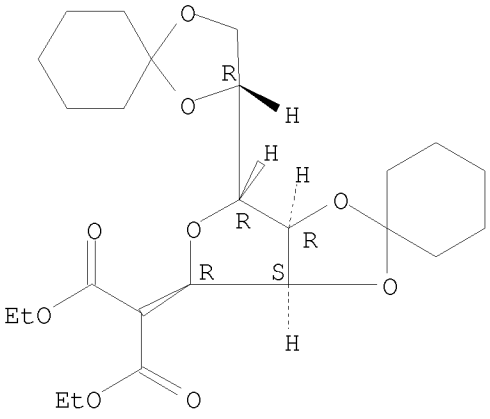
AB Glycosyl malonates I [R1 = CH(CO2Et)2, R2 = OH] and II [R1 = R2 = CH(CO2Et)2] were prepared in 80 and 60% yields by treatment of the corresponding ketones I, II (R1R2 = O) with BrCH(CO2Et)2. Similarly, III [R = CH(CO2Et)2] was prepared in 85% yield from III (R = OH).

IT 66295-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66295-09-8 CAPLUS

CN Propanedioic acid, (2,3:5,6-di-O-cyclohexylidene-α-D-mannofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:423653 CAPLUS

DOCUMENT NUMBER: 87:23653

ORIGINAL REFERENCE NO.: 87:3765a,3768a

TITLE: A rationalization on the relative thermodynamic stabilities of fused five-membered tetrahydrofurans with epimerizable substituents. An anomeric effect in furanoses

AUTHOR(S): Ohrui, Hiroshi; Emoto, Sakae

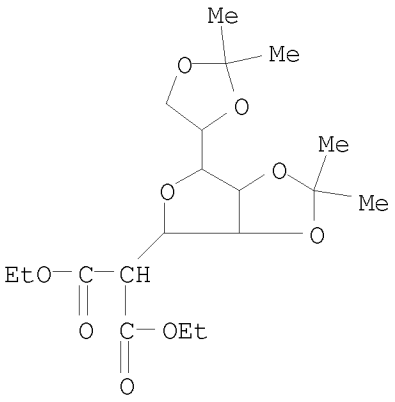
CORPORATE SOURCE: Inst. Phys. Chem. Res., Wako, Japan

SOURCE: Journal of Organic Chemistry (1977), 42(11), 1951-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

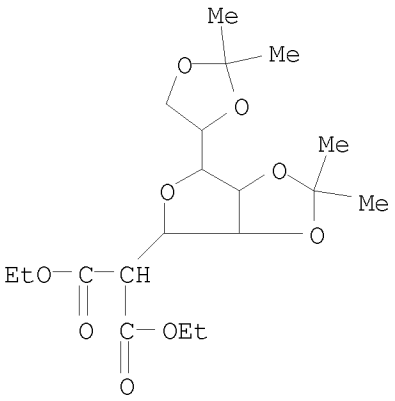
AB The thermodynamically more stable isomers of fused five-membered tetrahydrofuran derivs. with epimerizable substituents are the endo isomers. The fact that 2,3-O-isopropylidene or benzylidene furanoses exist mainly in the trans C-1,C-2 configuration should be explained in terms of the anomeric effect.

IT 52921-55-8 52921-56-9 56703-37-8
56703-38-9 56781-37-4 56781-38-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(1H NMR of, conformation in relation to)

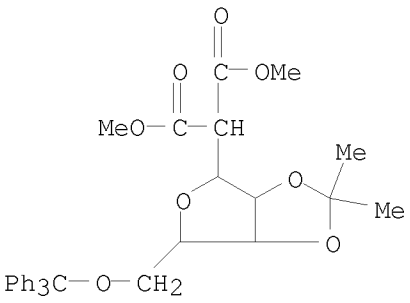
RN 52921-55-8 CAPLUS
CN Propanedioic acid, [2,3:5,6-bis-O-(1-methylethylidene)-α-D-mannofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



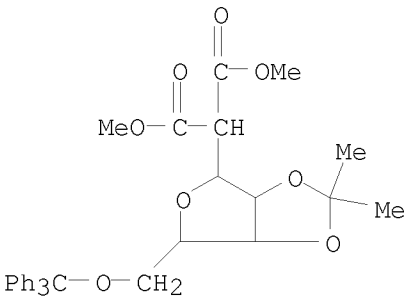
RN 52921-56-9 CAPLUS
CN Propanedioic acid, [2,3:5,6-bis-O-(1-methylethylidene)-β-D-mannofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



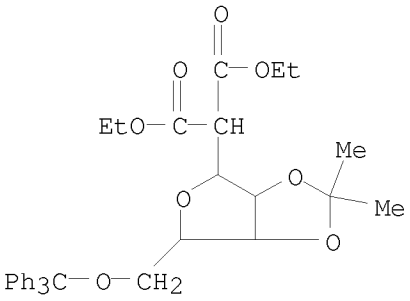
RN 56703-37-8 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



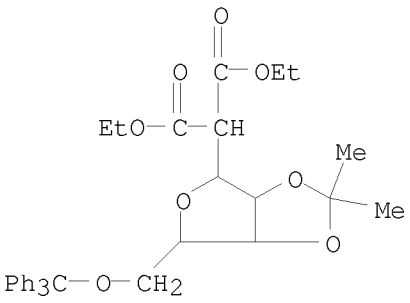
RN 56703-38-9 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



RN 56781-37-4 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



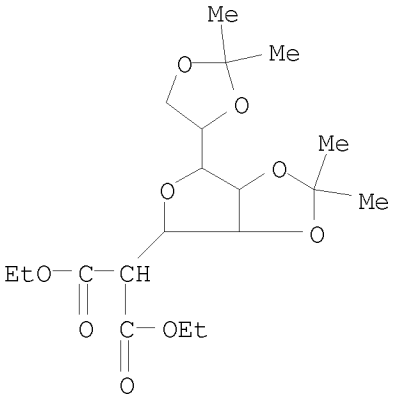
RN 56781-38-5 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



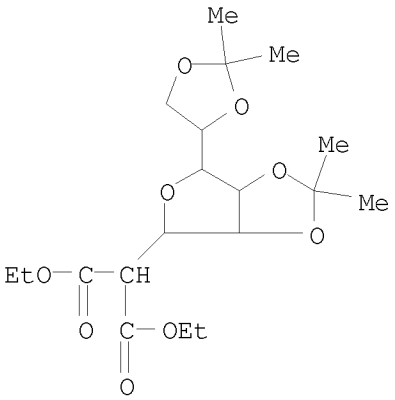
L12 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:514802 CAPLUS
DOCUMENT NUMBER: 83:114802
ORIGINAL REFERENCE NO.: 83:18055a,18058a
TITLE: C-Glycosyl nucleosides. V. Unexpected observations on the relative stabilities of compounds containing fused five-membered rings with epimerizable substituents
AUTHOR(S): Ohrui, Hiroshi; Jones, Gordon H.; Moffatt, John G.; Maddox, Michael L.; Christensen, Arild T.; Byram, Susan K.
CORPORATE SOURCE: Inst. Mol. Biol., Syntex Res., Palo Alto, CA, USA
SOURCE: Journal of the American Chemical Society (1975), 97(16), 4602-13
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reactions of 2,3-O-isopropylidene sugars with stabilized ylides lead to the formation of furanosyl C-glycosides in quantitative yield. By a combination of proton and 13C NMR spectroscopy, it was shown that the predominant kinetic product in each case was the isomer in which the introduced group was trans to the isopropylidene function. Base-catalyzed equilibration of these C-glycosides leads, to the cis C1 substituent and the isopropylidene function. Several 2-(2,3-O-isopropylidene-D-aldofuranosyl) malonates were also prepared by condensation of the appropriate aldofuranosyl halides with sodiomalonates. The kinetic and thermodyn. products have similarly been shown to have the malonate and isopropylidene functions oriented in a trans and cis fashion, resp. Condensation of 2,3,5-tri-O-benzyl-D-ribose with carbomethoxymethylenetriphenylphosphorane leads to a mixture of cis and trans olefins which rapidly cyclize to furanoxyl C-glycosides only upon treatment with base.

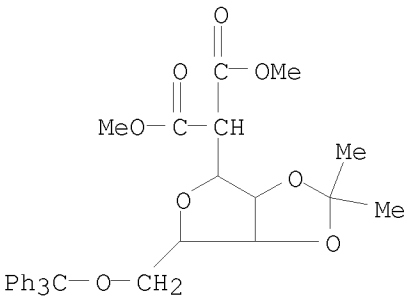
IT 52921-55-8P 52921-56-9P 56703-37-8P
56703-38-9P 56781-37-4P 56781-38-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 52921-55-8 CAPLUS
CN Propanedioic acid, [2,3:5,6-bis-O-(1-methylethylidene)-α-D-mannofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



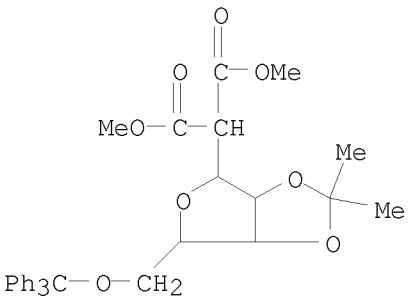
RN 52921-56-9 CAPLUS
CN Propanedioic acid, [2,3:5,6-bis-O-(1-methylethylidene)-β-D-mannofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



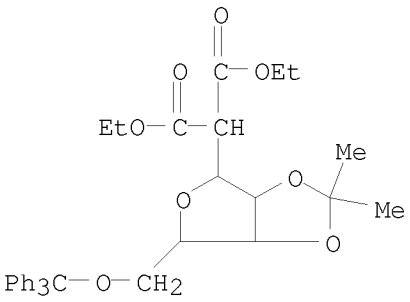
RN 56703-37-8 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



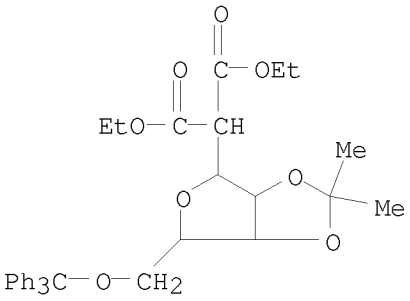
RN 56703-38-9 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, dimethyl ester (9CI) (CA INDEX NAME)



RN 56781-37-4 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

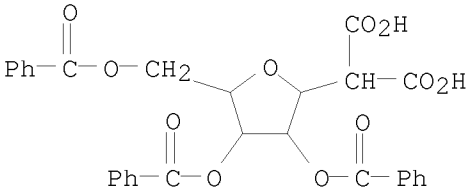


RN 56781-38-5 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-α-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

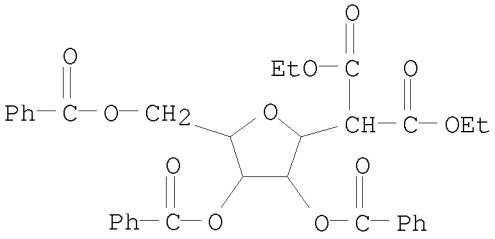


L12 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:410657 CAPLUS
DOCUMENT NUMBER: 83:10657
ORIGINAL REFERENCE NO.: 83:1801a,1804a
TITLE: Preparative and exploratory carbohydrate chemistry. Facile access to ethyl 2-C-β-D-ribofuranosylacetates
AUTHOR(S): Hanessian, Stephen; Ogawa, Tomoya; Guindon, Yvan
CORPORATE SOURCE: Dep. Chem., Univ. Montreal, Montreal, QC, Can.
SOURCE: Carbohydrate Research (1974), 38, C12-C14
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal

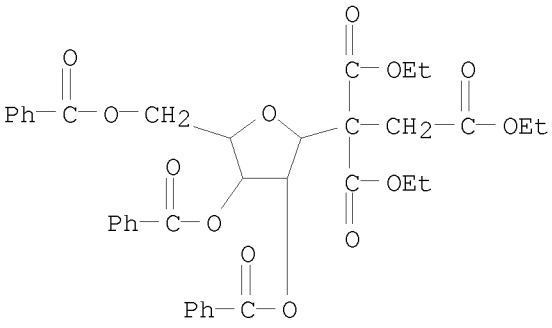
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Ph3P:CHCO2Et in boiling PhMe converted 2,3-O-isopropylidene-D-ribofuranose into Et 2-C-(2,3-O-isopropylidene-β-D-ribofuranosyl)acetate (I) and the 2,3,5-tri-O-benzoyl analog (II) was similarly prepared; the α-D anomer of II was prepared by thermal decarboxylation of 2-C-β-D-ribofuranosylmalonic acid, followed by esterification.
IT 50908-03-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decarboxylation of)
RN 50908-03-7 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)



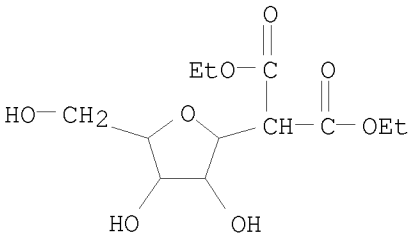
L12 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:413727 CAPLUS
DOCUMENT NUMBER: 81:13727
ORIGINAL REFERENCE NO.: 81:2219a,2222a
TITLE: Carbanions of carbohydrate chemistry. Approaches to chemical precursors of C-nucleosides
AUTHOR(S): Hanessian, Stephen; Pernet, Andre G.
CORPORATE SOURCE: Dep. Chem., Univ. Montreal, Montreal, QC, Can.
SOURCE: Canadian Journal of Chemistry (1974), 52(8, Pt. 1), 1280-93
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The condensation of D-ribofuranosyl halides containing participating, benzoate and nonparticipating, benzyl substituents, with sodio dialkyl malonates and sodio triethyl 1,1,2-ethanetricarboxylate is described. In the presence of participating groups at C-2, the major and sometimes exclusive products were the 1,2-acetal derivs. Both α- and β-anomeric D-ribofuranosyl malonates were formed in the non-participating series. Similar results were obtained with the more highly functionalized tricarbethoxy carbanion. For the participating series however, 20% of C-glycoside was obtained. Condensations with sodio diethyl malonate were also done in the D-arabino series with O-benzyl protecting groups and the anomeric C-glycosyl compds. were isolated and characterized.
IT 50907-70-5P 50907-72-7P 50907-91-0P 50907-92-1P 50907-93-2P 50907-94-3P 50907-97-6P 50907-98-7P 50907-99-8P 50908-00-4P 51094-92-9P 52950-03-5P 52950-04-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50907-70-5 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



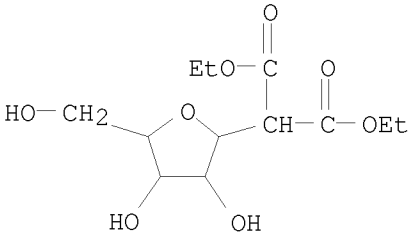
RN 50907-72-7 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, triethyl ester (9CI) (CA INDEX NAME)



RN 50907-91-0 CAPLUS
CN Propanedioic acid, α-D-ribofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)

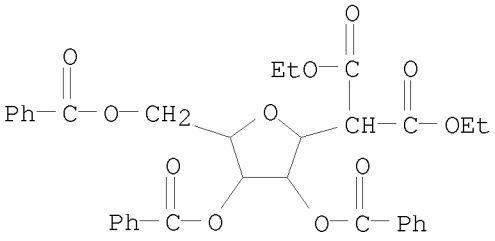


RN 50907-92-1 CAPLUS
CN Propanedioic acid, β-D-ribofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)

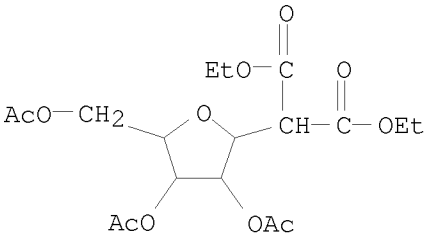


RN 50907-93-2 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-α-D-ribofuranosyl)-, diethyl

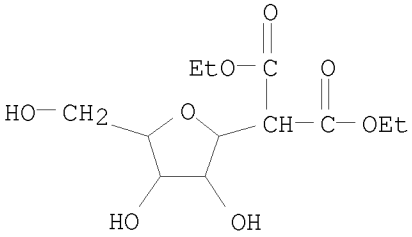
ester (9CI) (CA INDEX NAME)



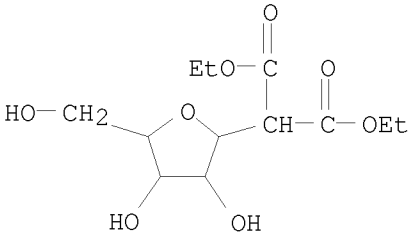
RN 50907-94-3 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 50907-97-6 CAPLUS
CN Propanedioic acid, α-D-arabinofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)

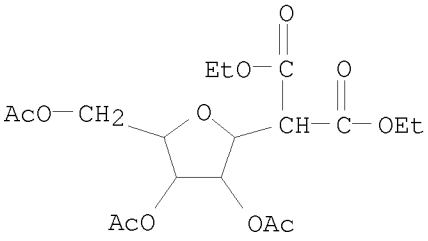


RN 50907-98-7 CAPLUS
CN Propanedioic acid, β-D-arabinofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)

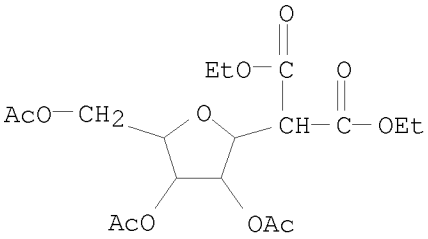


RN 50907-99-8 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-α-D-arabinofuranosyl)-,

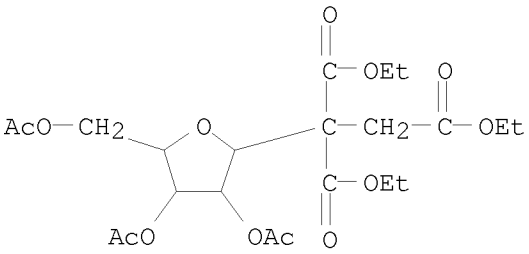
diethyl ester (9CI) (CA INDEX NAME)



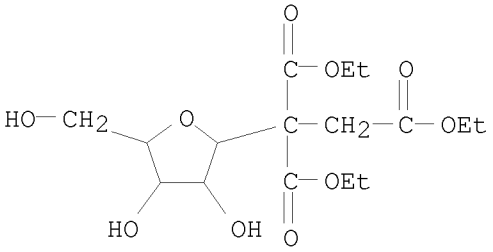
RN 50908-00-4 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-β-D-arabinofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 51094-92-9 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, triethyl ester (9CI) (CA INDEX NAME)

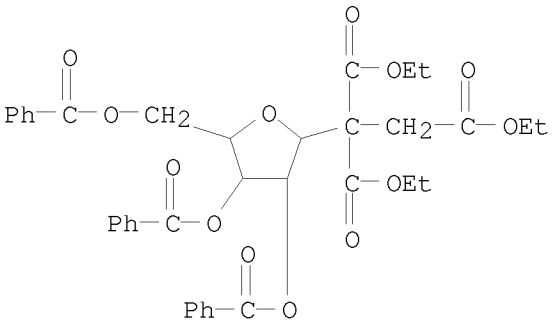


RN 52950-03-5 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-α-D-ribofuranosyl-, triethyl ester (9CI) (CA INDEX NAME)

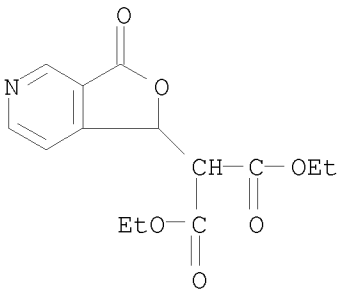


RN 52950-04-6 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-(2,3,5-tri-O-benzoyl-α-D-

ribofuranosyl)-, triethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:120704 CAPLUS
DOCUMENT NUMBER: 80:120704
ORIGINAL REFERENCE NO.: 80:19427a,19430a
TITLE: Pyrindine chemistry. II. Synthesis of 5,6-dihydro-2-pyrindin-7-one
AUTHOR(S): Binder, D.
CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Wien, Vienna, Austria
SOURCE: Monatshefte fuer Chemie (1974), 105(1), 196-202
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The pyrindinone I (R = H) was prepared by treating 3,4-pyridinedicarboxylic anhydride with H2C(CO2Et)2, reductive cleavage of the furopyridine II to III (R1 = CO2Et, R2 = Et), which was hydrolyzed to the acid and decarboxylated to III (R1 = R2 = H), whose Me ester was cyclized to I (R = CO2Me) and decarboxylated to.
IT 51907-11-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51907-11-0 CAPLUS
CN Propanedioic acid, (1,3-dihydro-3-oxofuro[3,4-c]pyridin-1-yl)-, diethyl ester (9CI) (CA INDEX NAME)

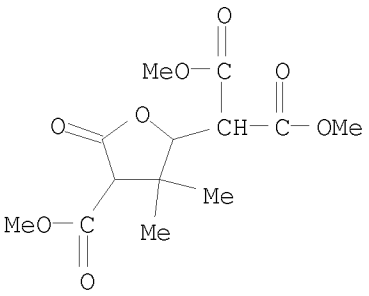


L12 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:14516 CAPLUS
DOCUMENT NUMBER: 80:14516

ORIGINAL REFERENCE NO.: 80:2441a,2444a
TITLE: Chemistry of α-haloaldehydes. III. Reaction of 2-halo-2-methylpropanal with malonic esters in the presence of potassium carbonate. (Synthesis of γ-butyrolactones)
AUTHOR(S): Takeda, Akira; Tsuboi, Sadao; Oota, Yasutsugu
CORPORATE SOURCE: Sch. Eng., Okayama Univ., Okayama, Japan
SOURCE: Journal of Organic Chemistry (1973), 38(24), 4148-52
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 80:14516

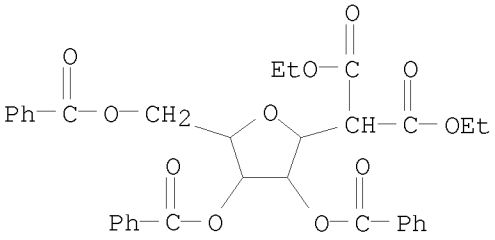
AB A new method for the preparation of γ-butyrolactone was described. 2-Chloro-2-methylpropanal (I) reacted with CH2(CO2R)2 in the presence of K2CO3 under mild conditions to give γ-butyrolactone derivs. in good yields. The reaction of I with CH2(CO2Me)2 in THF gave a mixture of Me 3-formyl-2-methoxycarbonyl-3-methylbutanoate (II) and α-methoxycarbonyl-β,β-dimethyl-γ-dimethoxycarbonylmethyl-γ-butyrolactone (III). The yield of III was greatly improved when 2 equivalent of CH2(CO2Me)2 in THF were used. Treatment of II with MeONa gave α-methoxycarbonyl-β,β-dimethyl-γ-methoxy-γ-butyrolactone, with NaCH(CO2Me)2 gave III. II treated with 2 equivalent of CH2(CO2Me)2 in aqueous K2CO3 gave predominantly α-methoxycarbonyl-β-dimethoxycarbonylmethyl-γ,γ-dimethyl-γ-butyrolactone which, hydrolyzed by concentrated HCl gave α-carboxy-β-carboxymethyl-γ,γ-dimethyl-γ-butyrolactone, which was decarboxylated to dl-terpenylic acid by heating.

IT 42203-06-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42203-06-5 CAPLUS
CN Propanedioic acid, [tetrahydro-4-(methoxycarbonyl)-3,3-dimethyl-5-oxo-2-furanyl]-, dimethyl ester (9CI) (CA INDEX NAME)

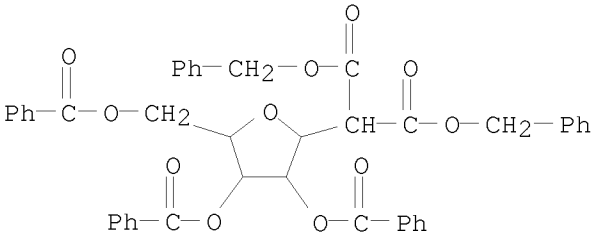


L12 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:3726 CAPLUS
DOCUMENT NUMBER: 80:3726
ORIGINAL REFERENCE NO.: 80:655a,658a
TITLE: New methods of anomeric C-functionalization. Route to the chemical precursors of C-nucleosides
AUTHOR(S): Ogawa, Tomoya; Pernet, Andre G.; Hanessian, Stephen
CORPORATE SOURCE: Dep. Chim., Univ. Montreal, Montreal, QC, Can.
SOURCE: Tetrahedron Letters (1973), (37), 3543-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal

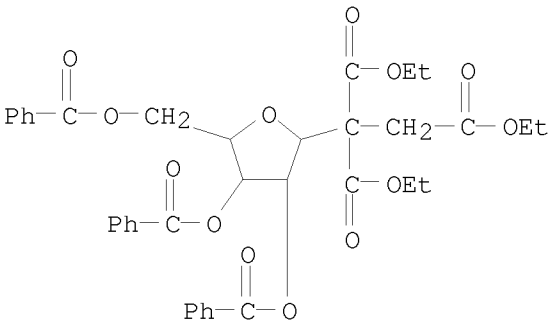
LANGUAGE: French
OTHER SOURCE(S): CASREACT 80:3726
GI For diagram(s), see printed CA Issue.
AB Treatment of the acetate (I) in CH_2Cl_2 with $SnCl_4$ followed by cyclohexanone enol trimethylsilyl ether gave the ribofuranosylcyclohexanone (II). Similar reaction with $RO_2C-CR1:C(OR)OSiMe_3$ (R = $SiMe_3$, CH_2Ph, R1 = H) gave ribofuranosyl derivs. (III, R = H, CH_2Ph, R1 = H), which were converted to III (R = Et, R1 = H), and I with $EtO_2CCH_2C-(CO_2Et):C(OEt)OSiMe_3$ gave III (R = Et, R1 = CH_2CO_2Et). I with $SnCl_4$ and 1-hexene followed by treatment of the product with $KMnO_4$-KIO_4-aqueous Me_2CO gave the acid IV. Bromination of III (R = Et, R1 = H) gave III (R = Et, R1 = Br).
IT 50907-70-5P 50907-71-6P 50907-72-7P
50907-73-8P 50907-79-4P 51094-92-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50907-70-5 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



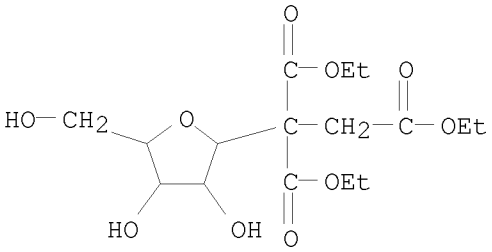
RN 50907-71-6 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)



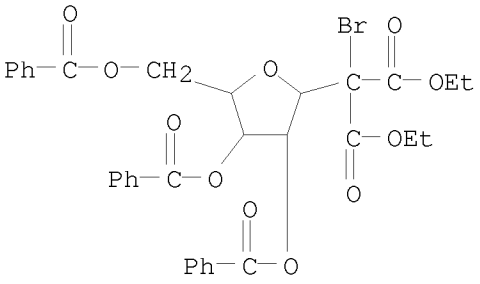
RN 50907-72-7 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, triethyl ester (9CI) (CA INDEX NAME)



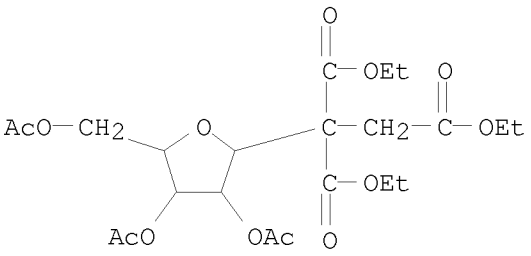
RN 50907-73-8 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-β-D-ribofuranosyl-, triethyl ester (9CI) (CA INDEX NAME)



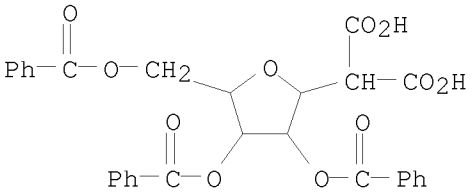
RN 50907-79-4 CAPLUS
CN Propanedioic acid, bromo(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



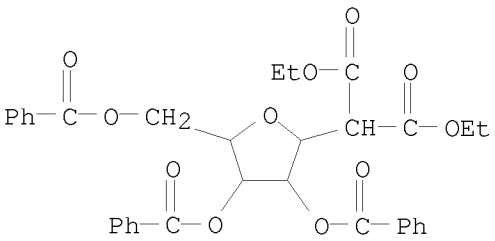
RN 51094-92-9 CAPLUS
CN 1,1,2-Ethanetricarboxylic acid, 1-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, triethyl ester (9CI) (CA INDEX NAME)



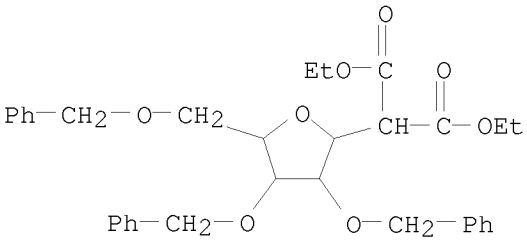
L12 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:3725 CAPLUS
DOCUMENT NUMBER: 80:3725
ORIGINAL REFERENCE NO.: 80:655a,658a
TITLE: Synthesis, anomeric assignation, and epimerization of the C-pentofuranosylmalonates
AUTHOR(S): Pernet, Andre G.; Ogawa, Tomoya; Hanessian, Stephen
CORPORATE SOURCE: Dep. Chim., Univ. Montreal, Montreal, QC, Can.
SOURCE: Tetrahedron Letters (1973), (37), 3547-50
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The ribofuranosyl chloride I (R = CH2Ph, R1 = Cl) with NaCH(CO2Et)2 in MeO(CH2)2OMe at 25° gave a mixture, containing I [R = CH2Ph, R1 = CH(CO2Et)2] and its α-anomer, which was hydrogenated and separated by chromatog. Periodate oxidation of I [R = H, R1 = CH(CO2Et)2] confirmed its β configuration. 2,3,5-Tri-O-benzyl-α-D-arabinofuranosyl chloride reacted similarly. Condensation of I (R = Bz, R1 = Br) with NaCH(CO2Et)2 in CH2(CO2Et)2 gave the oxepane II which formed by further reaction of the C-glycoside. Heating I [R = Bz, R1 = CH(CO2H)2] in AcOH followed by esterification gave a 1:1 mixture of I (R = Bz, R1 = CH2CO2Et) and its anomer.
IT 50908-03-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(decarboxylation and epimerization of)
RN 50908-03-7 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)



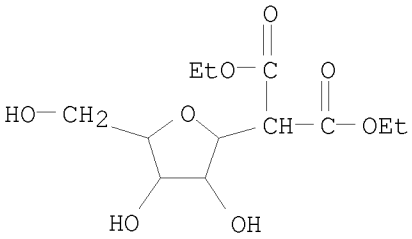
IT 50907-70-5P 50907-90-9P 50907-91-0P
50907-92-1P 50907-93-2P 50907-94-3P
50907-95-4P 50907-96-5P 50907-97-6P
50907-98-7P 50907-99-8P 50908-00-4P
51094-93-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50907-70-5 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



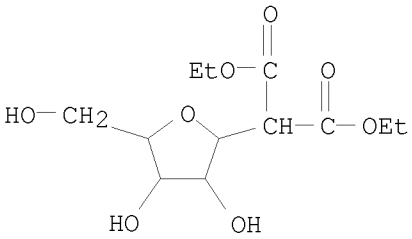
RN 50907-90-9 CAPLUS
CN Propanedioic acid, [2,3,5-tris-O-(phenylmethyl)-α-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



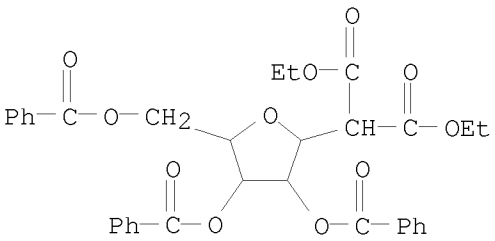
RN 50907-91-0 CAPLUS
CN Propanedioic acid, α-D-ribofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)



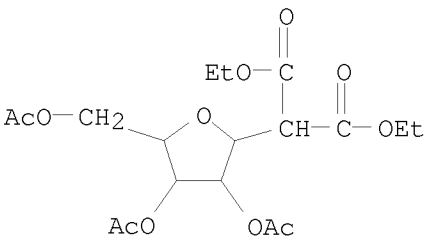
RN 50907-92-1 CAPLUS
CN Propanedioic acid, β-D-ribofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)



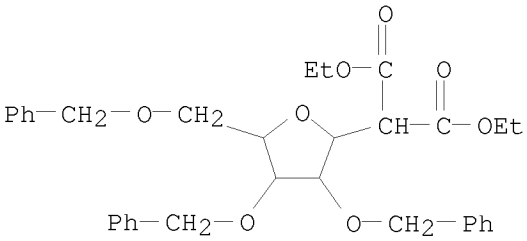
RN 50907-93-2 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-benzoyl-α-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



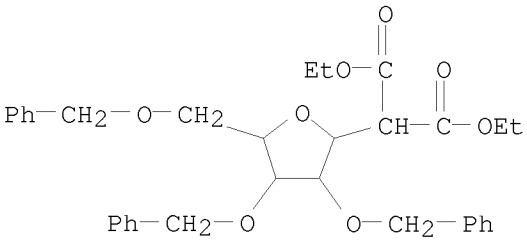
RN 50907-94-3 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



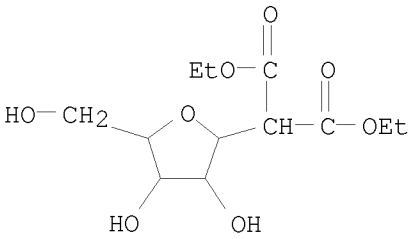
RN 50907-95-4 CAPLUS
CN Propanedioic acid, [2,3,5-tris-O-(phenylmethyl)-β-D-arabinofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



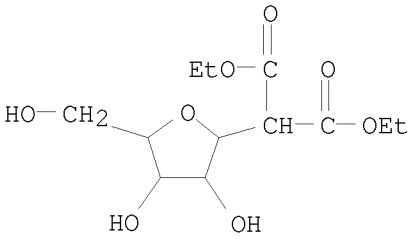
RN 50907-96-5 CAPLUS
CN Propanedioic acid, [2,3,5-tris-O-(phenylmethyl)-α-D-arabinofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)



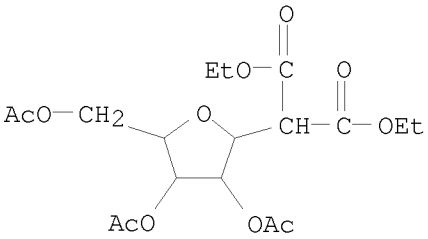
RN 50907-97-6 CAPLUS
CN Propanedioic acid, α-D-arabinofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)



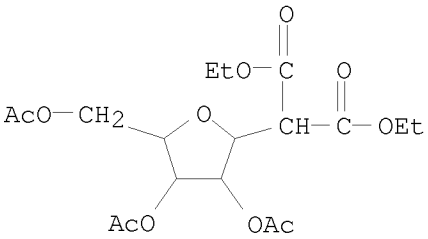
RN 50907-98-7 CAPLUS
CN Propanedioic acid, β-D-arabinofuranosyl-, diethyl ester (9CI) (CA INDEX NAME)



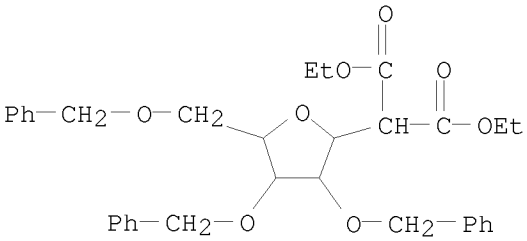
RN 50907-99-8 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-α-D-arabinofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



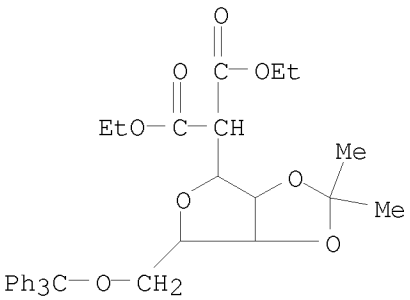
RN 50908-00-4 CAPLUS
CN Propanedioic acid, (2,3,5-tri-O-acetyl-β-D-arabinofuranosyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 51094-93-0 CAPLUS
CN Propanedioic acid, [2,3,5-tris-O-(phenylmethyl)-β-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

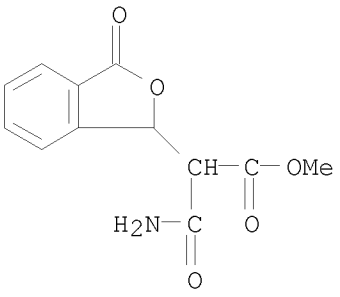


L12 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:479125 CAPLUS
DOCUMENT NUMBER: 79:79125
ORIGINAL REFERENCE NO.: 79:12853a,12856a
TITLE: Nucleosides. LXXXI. Approach to the synthesis of C-C linked β-D-ribofuranosyl nucleosides from 2,3-O-isopropylidene-5-O-trityl-β-D-ribofuranosyl chloride
AUTHOR(S): Ohrui, Hiroshi; Fox, Jack J.
CORPORATE SOURCE: Mem. Sloan-Kettering Cancer Cent., Cornell Univ., New York, NY, USA
SOURCE: Tetrahedron Letters (1973), (22), 1951-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2,3-O-Isopropylidene-5-O-trityl-β-D-ribosyl chloride (I, R = Cl) was obtained by reaction of 2,3-O-isopropylidene-D-ribofuranose with Ph3CCl and then with Ph3P-CCl4. I condensed with NaCH(CO2Et)2-NaI to give di-Et 2,3-O-isopropylidene-5-O-trityl-D-ribofuranosyl malonate (II, R = OEt), the α:β ratio of which depended on reflux time. Treatment of II (R = OEt) with urea-EtONa gave I (R = Na barbiturate). Treatment of I (R = Cl) with MeCOCHNaCO2Et gave II (R = Me) and the O-glycoside (III).
IT 49561-16-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 49561-16-2 CAPLUS
CN Propanedioic acid, [2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-D-ribofuranosyl]-, diethyl ester (9CI) (CA INDEX NAME)

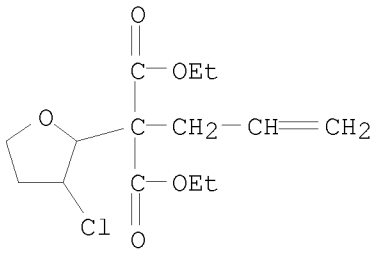


L12 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:16008 CAPLUS
DOCUMENT NUMBER: 78:16008
ORIGINAL REFERENCE NO.: 78:2535a,2538a

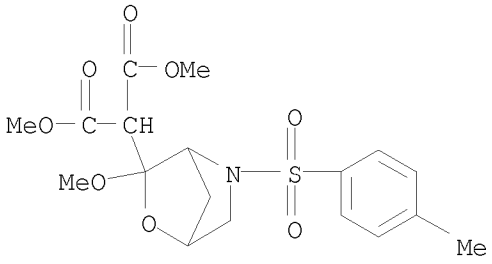
TITLE: Synthesis of 2-benzazepine-1,3-diones and corresponding 4,5-dihydro compounds
AUTHOR(S): Walker, Gordon N.
CORPORATE SOURCE: Pharm. Div., Ciba-Geigy Corp., Summit, NJ, USA
SOURCE: Journal of Organic Chemistry (1972), 37(24), 3955-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 78:16008
AB The title compound was obtained by cyclization of cis-cinnamonitrile-o-carboxylic acid. Condensation of phthalaldehydic acid with active methylene compds. gave a series of α-substituted β-(o-carboxyphenyl)propionitrile derivs.
IT 36004-44-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36004-44-1 CAPLUS
CN 1-Isobenzofuranacetic acid, α-(aminocarbonyl)-1,3-dihydro-3-oxo-, methyl ester (CA INDEX NAME)



L12 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:448109 CAPLUS
DOCUMENT NUMBER: 77:48109
ORIGINAL REFERENCE NO.: 77:7967a,7970a
TITLE: Synthesis of allyl-β-chlorotetrahydrofurylmalonic ester and its chemical reactions
AUTHOR(S): Mesropyan, E. G.; Egikyan, M. G.; Dangyan, M. T.
CORPORATE SOURCE: Erevan. Gos. Univ., Erevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1972), 25(2), 137-9
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Reaction of di-Et allylmalonate with 2,3-dichlorotetrahydrofuran gave di-Et (3-chlorotetrahydro-2-furyl)allylmalonate (I). Oxidation of I with H2O2 in Ac2O gave II (R = OH). Another γ-valerolactone derivative II (R = Br) was obtained by bromination of I followed by distillation in vacuo.
IT 36842-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36842-67-8 CAPLUS
CN Propanedioic acid, (3-chlorotetrahydro-2-furanyl)-2-propenyl-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:509496 CAPLUS
DOCUMENT NUMBER: 75:109496
ORIGINAL REFERENCE NO.: 75:17295a,17298a
TITLE: Bicyclic bases. Ambident anions as intramolecular nucleophiles in the formation of 2-oxa-5-azabicyclo[2.2.1] heptane derivatives
AUTHOR(S): Portoghese, P. S.; Sepp, D. T.
CORPORATE SOURCE: Coll. Pharm., Univ. Minnesota, Minneapolis, MN, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(4), 531-5
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 75:109496
AB The intramol. cyclization of the ambident anion derived from condensation of N,O-ditosylhydroxy-L-proline acid chloride with di-Me malonate anion was studied under a variety of reaction conditions. Cyclization occurred solely by O-alkylation to give 2-oxa-5-azabicyclo[2.2.1]heptanes. The NMR spectra of the bicyclo compds. are discussed.
IT 33812-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33812-97-4 CAPLUS
CN 2-Oxa-5-azabicyclo[2.2.1]heptane-3-malonic acid, 3-methoxy-1-(p-tolylsulfonyl)-, (+)- (8CI) (CA INDEX NAME)



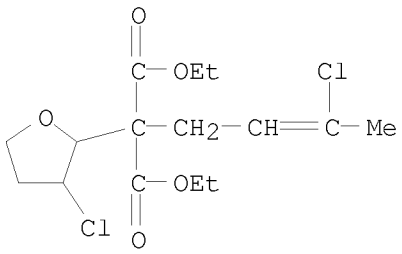
L12 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:435561 CAPLUS
DOCUMENT NUMBER: 75:35561
ORIGINAL REFERENCE NO.: 75:5613a,5616a
TITLE: Synthesis of new derivatives of tetrahydrofuran. III
AUTHOR(S): Mesropyan, E. G.; Bunyatyan, Yu. A.; Karapetyan, Z. T.; Dangyan, M. T.
CORPORATE SOURCE: Erevan. Gos. Univ., Erevan, USSR

SOURCE: Armyanskii Khimicheskii Zhurnal (1971), 23(12), 1103-7
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian

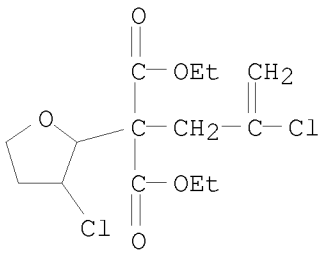
AB Reaction of α,β-dichlorotetrahydrofuran with di-Et (β-chloroallyl)-, (γ-chlorocrotyl)-, or isoamylmalonate and Na in Et2O gave 26.4% di-Et (β-chlorotetrahydrofuryl)(β-chloroallyl)malonate and 72.5% of its oligomer; 66.2% di-Et (β-chlorotetrahydrofuryl)(γ-chlorocrotyl)malonate (I) and 16.6% oligomer; and 68.7% di-Et (β-chlorotetrahydrofuryl)isoamylmalonate and 23% oligomer. Cyclization of I with Ac2O and H2O2 gave 76.5% α-(ethoxy carbonyl)-α-(β-chlorotetrahydrofuryl)-γ-acetyl-γ-butyrolactone. Furan ring opening occured by refluxing di-Et (β-chlorotetrahydrofuryl)malonate with Na in Et2O, and di-Et butyl(4-hydroxy-1-butenyl)malonate (II) was formed in 62.3% yield. Addition of Br to II in CCl4 gave 69.6% α-butyl-α-(ethoxycarbonyl)-β-bromo-γ-(β-hydroxyethyl)-γ-butyrolactone and di-Et butyl(1,2-dibromo-4-hydroxybutyl)malonate.

IT 24866-19-1P 27223-51-4P 32561-04-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

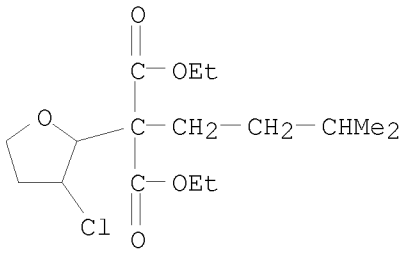
RN 24866-19-1 CAPLUS
CN 2-Furanmalonic acid, 3-chloro-α-(3-chloro-2-butenyl)tetrahydro-, diethyl ester (8CI) (CA INDEX NAME)



RN 27223-51-4 CAPLUS
CN 2-Furanmalonic acid, 3-chloro-α-(2-chloroallyl)tetrahydro-, diethyl ester (8CI) (CA INDEX NAME)



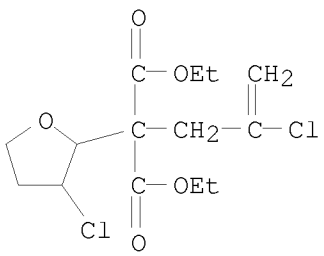
RN 32561-04-9 CAPLUS
CN 2-Furanmalonic acid, 3-chlorotetrahydro-α-isopentyl-, diethyl ester (8CI) (CA INDEX NAME)



L12 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:132492 CAPLUS
DOCUMENT NUMBER: 72:132492
ORIGINAL REFERENCE NO.: 72:23711a,23714a
TITLE: Diethyl ester of β-chlorotetrahydrofuryl-β-chloroallylmalonic acid
INVENTOR(S): Mesropyan, E. G.; Avetisyan, A. A.; Shaginyan, A. O.; Dangyan, M. T.
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1969, 46(35), 23.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 256751		19691111	SU	19661206 <--

AB The title compound is prepared by treating α,β-dichlorotetrahydrofuran with diethyl β-chloroallylmalonate at elevated temperature in absolute Et2O in the presence of metallic Na.
IT 27223-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27223-51-4 CAPLUS
CN 2-Furanmalonic acid, 3-chloro-α-(2-chloroallyl)tetrahydro-, diethyl ester (8CI) (CA INDEX NAME)

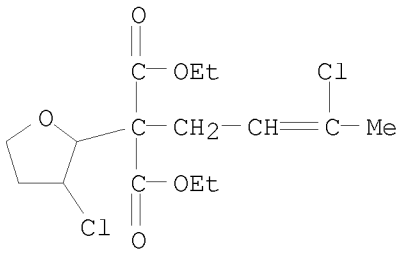


L12 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:3347 CAPLUS
DOCUMENT NUMBER: 72:3347
ORIGINAL REFERENCE NO.: 72:603a,606a
TITLE: Diethyl β-chlorotetrahydrofuryl-γ-chlorocrotylmalonate
INVENTOR(S): Mesropyan, E. G.; Avetisyan, A. A.; Dangyan, M. T.;

Egikyan, M. G.
PATENT ASSIGNEE(S): Erevan State University
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1969, 46(19), 24.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 245069		19690604	SU	19680401 <--

AB The title ester is obtained by treating α,β-dichlorotetrahydrofuran with the diethyl γ-chlorocrotylmalonate in the presence of metallic Na in an organic solvent, such as Et2O, at the b.p. of the reaction mixture, with subsequent separation of the desired product.
IT 24866-19-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24866-19-1 CAPLUS
CN 2-Furanmalonic acid, 3-chloro-α-(3-chloro-2-butenyl)tetrahydro-, diethyl ester (8CI) (CA INDEX NAME)

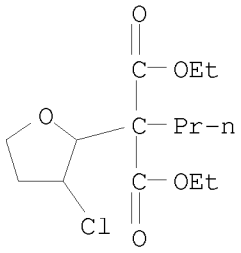


L12 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:481057 CAPLUS
DOCUMENT NUMBER: 71:81057
ORIGINAL REFERENCE NO.: 71:15001a
TITLE: New tetrahydrofuran derivatives
AUTHOR(S): Mesropyan, E. G.; Avetisyan, A. A.; Dangyan, M. T.; Buniatyan, Yu. A.
CORPORATE SOURCE: Erevan. Gos. Univ., Erevan, USSR
SOURCE: Armyanskii Khimicheskii Zhurnal (1969), 22(3), 231-3
CODEN: AYKZAN; ISSN: 0515-9628
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB α,β-Dichlorotetrahydrofuran (I) reacted with Na derivs. of RCH(CO2Et)2 (R = H, Pr, or Bu) in absolute Et2O to give 3-chlorotetrahydrofur-2-yl malonates. Thus, 160 g. CH2(CO2Et)2 was added to a flask containing 23 g. Na and 250 ml. Et2O. The mixture was cooled and 141 g. I was added dropwise. The salt formed after refluxing the mixture for 2 hrs. was dissolved in H2O, and the ether layer separated and dried over Na2SO4. After vacuum distillation, 65 g. di-Et β-chlorotetrahydrofur-2-ylmalonate (II) was obtained; b1 130-40°, n20D 1.4608. Similar preparation conducted in the presence of SbCl5 afforded 61% II and 38% of a polymer. Cognate prepns. involved reactions of I with di-Et propylmalonate to give di-Et

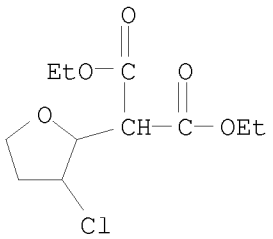
(3-chlorotetrahy-drofuryl)propylmalonate, b1 138-45°, n20D 1.4690. A residue in the distilling flask consisted of an oily, viscous polymer soluble in Me2CO. A reaction between I and di-Et butylmalonate gave di-Et 3-(chlorotetrahydrofur-2-yl)butylmalonate (III); (trans) b.p. 130-40°/1 mm., n20D 1.4598; and cis b.p. 140-9°/1 mm., n20D 1.4654. An oligomer was also obtained.

IT 19097-01-9P 22915-87-3P 24280-91-9P 24306-40-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19097-01-9 CAPLUS
CN 2-Furanmalonic acid, 3-chlorotetrahydro-α-propyl-, diethyl ester (8CI) (CA INDEX NAME)

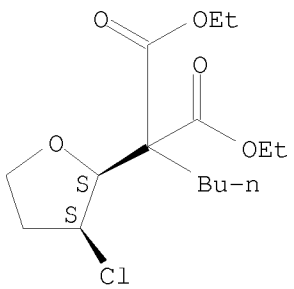


RN 22915-87-3 CAPLUS
CN 2-Furanmalonic acid, 3-chlorotetrahydro-, diethyl ester (8CI) (CA INDEX NAME)



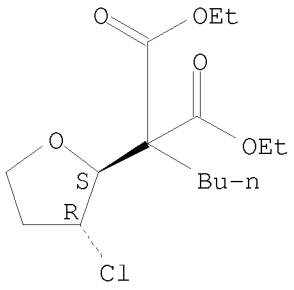
RN 24280-91-9 CAPLUS
CN 2-Furanmalonic acid, α-butyl-3-chlorotetrahydro-, diethyl ester, cis- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 24306-40-9 CAPLUS
CN 2-Furanmalonic acid, α-butyl-3-chlorotetrahydro-, diethyl ester, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L12 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:451977 CAPLUS
DOCUMENT NUMBER: 69:51977
ORIGINAL REFERENCE NO.: 69:9703a,9706a
TITLE: Diethyl β-chlorotetrahydrofurylpropylmalonate
INVENTOR(S): Mesropyan, E. G.; Avetisyan, A. A.; Shaginyan, A. O.; Dangyan, M. T.
SOURCE: U.S.S.R. From: Izobret., Prom. Obraztsy, Tovarnye Znaki 1968, 45(11), 36.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

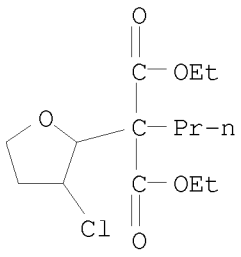
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 213894		19680320	SU	19661128 <--

AB The ester is prepared from the reaction of α,β-dichlorotetrahydrofuran with diethyl propylmalonate in the presence of metallic Na in a suitable organic solvent, e.g. Et2O, with heating.

IT 19097-01-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

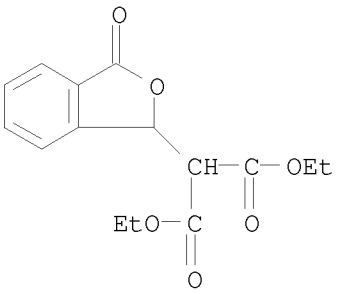
RN 19097-01-9 CAPLUS

CN 2-Furanmalonic acid, 3-chlorotetrahydro-α-propyl-, diethyl ester (8CI) (CA INDEX NAME)



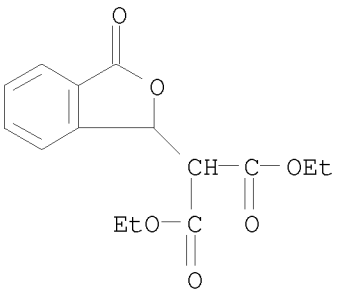
L12 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1967:421762 CAPLUS
DOCUMENT NUMBER: 67:21762
ORIGINAL REFERENCE NO.: 67:4131a
TITLE: Phthalyl- and phthalidylmalonic esters

AUTHOR(S): Suszko, Jerzy; Kinastowski, Stefan
CORPORATE SOURCE: Polska Akad. Nauk, Poznan, Pol.
SOURCE: Roczniki Chemii (1967), 41(1), 111-17
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: Polish
GI For diagram(s), see printed CA Issue.
AB A mixture of 2.5 g. dispersed metallic Na in 130 ml. anhydrous Et2O was treated successively, under cooling and stirring, with 17.3 g. CH2(CO2Et)2 and 10 g. I (R = R1 = Cl), then kept 5 hrs. at room temperature, refluxed 2 hrs., filtered, evaporated, and distilled in vacuo to remove diethyl malonate. The residue gave II, m. 74.5° (Et2O). A mixture of NaCH(CO2Et), prepared from 4 g. diethyl malonate and 1.15 g. dispersed metallic Na, in 200 ml. anhydrous benzene was treated with 5.3 g. III (R = Et, R1 = COCl), the mixture kept 4 hrs. at room temperature and filtered, and the organic layer washed with aqueous NaHCO3 and water, dried, and evaporated to give an oily residue. When dissolved in Et2O and shaken with aqueous CuSO4 the residue afforded III [R = Et, R1 = COCH(CO2Et)2] (IV) in the form of the Cu salt, m. 89° (80% EtOH). The salt acidified with HCl and extracted with Et2O gave IV. An ethereal solution of IV acidified with AcOH and kept a few weeks gave II. Hydrogenation of 2 g. II in a suspension of Raney W-7 Ni, prepared from 20 ml. catalyst in 50 ml. anhydrous benzene saturated with hydrogen, gave III [R = H, R1 = CH2CH(CO2Et)2], m. 88°, and V (R = R1 = CO2Et) (VI), m. 44° (petr. ether). A solution of III (R = Na, R1 = CHO), prepared from 5 g. III (R = H, R1 = CHO) in 15 ml. H2O and equimolar amount of NaOH, was treated with 5 g. diethyl malonate, 3 drops piperidine, and EtOH until the whole became homogeneous and the mixture kept 10 days at room temperature to give VI. VI was also prepared from 2 g. I (R = H, R1 = Cl) and NaCH(CO2Et)2 in 25 ml. anhydrous benzene. Hydrolysis of 0.5 g. VI with 0.5 g. KOH in 15 ml. H2O led to I (R = H, R1 = CH2CO2H), m. 101° (H2O), m. 152° (PhMe).
IT 7137-24-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 7137-24-8 CAPLUS
CN Propanedioic acid, (1,3-dihydro-3-oxo-1-isobenzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:420682 CAPLUS
DOCUMENT NUMBER: 65:20682
ORIGINAL REFERENCE NO.: 65:3819d-f
TITLE: Molecular structure and properties of diethyl phthalyl- and diethyl phthalidylmalonate

AUTHOR(S): Suszko, J.; Kinastowski, S.
CORPORATE SOURCE: A. Mickiewicz Univ., Poznan
SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (1966), 14(3), 157-61
CODEN: BAPCAQ; ISSN: 0001-4095
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Chemical and ir spectroscopic evidence was presented in favor of formula I suggested by Wislicenus (Ann. 242, 23(1887) for diethyl phthalylmalonate. The catalytic hydrogenation of I in dry C6H6 at room temperature proceeded with the consumption of 1.6 moles H/mole I and the formation of o-HO2CC6H4CH2CH(CO2Et)2 and II, m. 44° (petr. ether). I hydrolyzed with KOH and then acidified yielded oily phthalidylmalonic acid which upon partial decarboxylation gave phthalidylacetic acid. Chlorophthalide (IIb) condensed with NaCH(CO2Et)2 (III) gave II. o-NaO2CC6H4CHO condensed with CH2(CO2Et)2 in the presence of piperidine yielded II and o-NaO2CC6H4CH(OH)CH(CO2Et)2 (IV). II and IV apparently coexisted in an equilibrium under the reaction conditions. EtO2CC6H4COCl condensed with III yielded o-EtO2CC6H4COCH(CO2Et)2 (V) (Cu salt m. 89°), which upon acidification yielded II. V was identical with the product obtained by W. (loc. cit.) from I and NaOEt. Asym. IIb condensed readily with III to give I. On the other hand, sym. IIb reacted to yield I via the intermediate o-ClOCC6H4C(OH):C(CO2Et)2. The ir spectra of I and II are recorded.
IT 7137-24-8P, 1-Phthalanmalonic acid, 3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 7137-24-8 CAPLUS
CN Propanedioic acid, (1,3-dihydro-3-oxo-1-isobenzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)

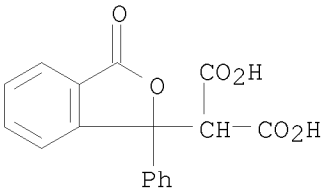


L12 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:79241 CAPLUS
DOCUMENT NUMBER: 56:79241
ORIGINAL REFERENCE NO.: 56:15420d-g
TITLE: Reaction of the cyclic chloride of o-benzoylbenzoic acid with diethyl (ethoxymagnesio)methylmalonate
AUTHOR(S): Newman, Melvin S.
CORPORATE SOURCE: Ohio State Univ., Columbus
SOURCE: Journal of Organic Chemistry (1962), 27, 323-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB CH2(CO2Et)2 (20 g.) in 50 ml. Et2O and 100 ml. (EtOCH2CH2)2O treated

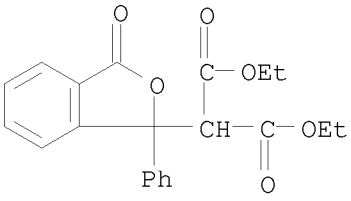
portionwise with 2.3 g. Na and the solution treated with 24.0 g. o-BzC6H4CO2Me in 25 ml. (EtOCH2CH2)2O, the Et2O evaporated and the mixture refluxed 6.5 hrs., the cooled mixture poured into ice and HCl and the neutral fraction of the product distilled yielded 14.0 g. o-BzC6H4CO2Me, b0.5 170-90°, and 12.0 g. yellow viscous material, b0.5 230-45°, crystallized from alc. to give 16% crystals, m. 95.0-8.6°, recrystd. to di-Et 3-phenylphthalidylmalonate (I), m. 100.4-1.8°, hydrolyzed in hot NaOH and acidified with HCl to give C6H6-insol. 3-phenylphthalidylmalonic acid (II), m. 160° (decomposition). Material prepared according to Bergmann (CA 33, 42257) and purified by alkaline hydrolysis to remove o-BzC6H4CO2Me gave pure 3-methyl-3-phenylphthalide (III), m. 76.8-8.0°, λ 5.65 μ II heated 20 min. at 200-5° and the product distilled in vacuo gave a good yield of III. The pseudo acid chloride [prepared from 50.0 g. o-BzC6H4CO2H according to Koelsch (CA 54, 18424e)] in 100 ml. dry Et2O refluxed 1-12 hrs. with EtOMgCMe(CO2Et)2 (from 5.4 g. Mg and 38.0 g. MeCH(CO2Et)2) and the cooled mixture treated with dilute HCl, taken up in Et2O-C6H6 and the warm solution washed with aqueous Na2CO3, concd, and the combined crops (81-86%, m. 103-7°) recrystd. from alc. gave di-Et 3-phenylphthalidylmethylmalonate (IV), m. 106-7°. Attempts to hydrolyze IV to the free acid resulted only in recovery of unchanged material or cleavage to o-BzC6H4CO2H. Whereas the ethoxymagnesio derivative displaced the Cl atom of the pseudo acid chloride, it was noteworthy that the ethoxymagnesio derivative of CH2(CO2Et)2 reacted by attack at the CO group to give the enol form of o-BzC6H4COCH(CO2Et)2.

IT 93328-26-8P, 1-Phthalanmalonic acid, 3-oxo-1-phenyl-
94875-82-8P, 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester 95137-09-0P, 1-Phthalanmalonic acid, α-methyl-3-oxo-1-phenyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)

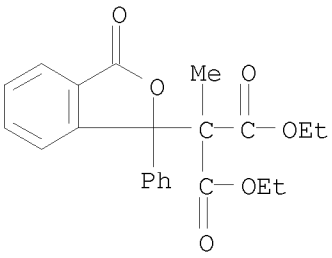
RN 93328-26-8 CAPLUS
CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl- (6CI, 7CI) (CA INDEX NAME)



RN 94875-82-8 CAPLUS
CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)



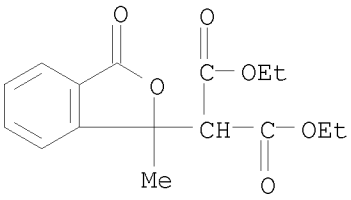
RN 95137-09-0 CAPLUS
CN 1-Phthalanmalonic acid, α-methyl-3-oxo-1-phenyl-, diethyl ester (7CI) (CA INDEX NAME)



L12 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:65087 CAPLUS
DOCUMENT NUMBER: 55:65087
ORIGINAL REFERENCE NO.: 55:12416f-i
TITLE: Preparation of aromatic monocarbonyl and o-dicarbonyl compounds. I. Aromatic o-acetylcarboxylic acids
AUTHOR(S): Ried, Walter; Bonnighausen, Karl Heinz
CORPORATE SOURCE: Univ. Frankfurt a. M., Germany
SOURCE: Justus Liebigs Annalen der Chemie (1961), 639, 56-60
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Phthalic anhydride was converted to the Me half ester, then to the ester acid chloride (not isolated). Treatment of the acid chloride with Mg(OEt)2 and CH2(CO2Et)2 (I) yielded di-Et o-carbomethoxybenzoylmalonate (85%). Acid hydrolysis resulted in o-acetylbenzoic acid (II, 60%, m. 115-7°). Similarly, 1,2-naphthalenedicarboxylic acid was converted to the Me ester acid chloride, which with I yielded di-Et 1-carbomethoxy-2-naphthoylmalonate (14%, m. 92.5-4.5°), and finally to 2-acetyl-1-naphthoic acid (III, 58%, m. 198.5-9.5°). 2,3-Naphthalenedicarboxylic acid with I gave di-Et 2-carbomethoxy-3-naphthoylmalonate (92%, m. 89-91°), which was converted to 3-acetyl-2-naphthoic acid (IV), 87.5%, m. 170-1°). Di-Et 2-carbomethoxy-3-pyridylcarbonylmalonate, m. 110° (decomposition), was prepared With NH2NH2, II yielded 1-hydroxy-4-methylphthalazine; IV yielded 6,7-benzo-1-hydroxy-4-methylphthalazine (97.5%, m. 280-2°); and III yielded the corresponding 5,6-benzophthalazone. II with PhNHNH2, or with p-NO2C6H4NHNH2, did not yield hydrazones, but phthalazones: 2-phenyl-4-methylphthalazone (81.5%, m. 98-9°) and 2-(p-nitrophenyl)-4-methylphthalazone (71%, m. 214-15°). Only with unsym. hydrazines were hydrazones obtained. II and MePhNNH2 gave the hydrazone (83%, m. 117-18°). II with SOCl2 gave the acid chloride, but failed to give di-Et o-acetylbenzoylmalonate with I. An indanone (or a phthalide) was suggested as the product.

IT 101432-32-0P, 1-Phthalanmalonic acid, 1-methyl-3-oxo-(?), diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 101432-32-0 CAPLUS
CN Propanedioic acid, (1,3-dihydro-1-methyl-3-oxo-1-isobenzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)

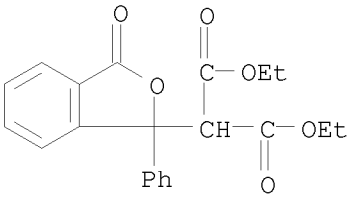


L12 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:97373 CAPLUS
DOCUMENT NUMBER: 54:97373
ORIGINAL REFERENCE NO.: 54:18424e-h
TITLE: Condensation or o-benzoylbenzoyl chloride with ethyl malonate
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of Organic Chemistry (1960), 25, 642-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:97373

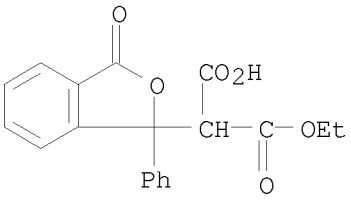
AB The compound formed by action of o-benzoylbenzoyl chloride (I) on ethoxy-magnesiomalonic ester was actually the enol form of Et o-benzoylbenzoylmalonate (II). It was not necessary to avoid heating I, and the product was freed of SOCl2 at 100° in vacuo. Since II was soluble in and rapidly altered by Na2CO3 an excess was avoided in the final washing of the crude product. Pure II m. 86-8° (EtOAc-ligroine). Na (10 g.) in 100 ml. alc. treated with 70 g. Et malonate and then 100 g. Et benzoylbenzoate, the mixture refluxed 1.5 hrs., distilled to a sirup, 400 ml. H2O added, and the mixture extracted with Et2O gave 9.1 g. Et malonate and 20 g. Et benzoylbenzoate. The product precipitated by acidification gave 95 g. Et 3-phenylphthalidylmalonate (III), m. 100-2° (EtOAc-ligroine). III refluxed with 10% Na2CO3 during 5 min. gave a colorless solution and acidification afforded an acid ester, m. 97-8° (EtOAc-ligroine). When 1 g. III was refluxed 1 hr. with 4 ml. AcOH and 4 ml. 48% HBr, it gave 3-phenylphthalide-3-acetic acid, m. 177-8° (PhMe). Refluxing the acid with MeOH-H2SO4 gave Me 3-phenylphthalide-3-acetate, needles, m. 86-7°. III (6.7 g.) refluxed 15 min. with 4 g. NaOH in 25 ml. H2O, the solution cooled, acidified, and the product isolated gave 5.3 g. 3-phenylphthalidylmalonic acid, m. 160-4°, resolidified, and m. 176-8° (Me2CO-ligroine).

IT 94875-82-8 111441-87-3
(Derived from data in the 6th Collective Formula Index (1957-1961))

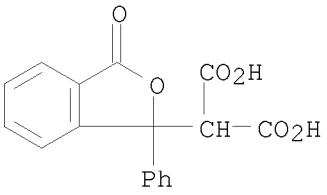
RN 94875-82-8 CAPLUS
CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)



RN 111441-87-3 CAPLUS
CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, ethyl ester (6CI) (CA INDEX NAME)



IT 93328-26-8P, 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, ethyl esters
RL: PREP (Preparation)
(preparation of)
RN 93328-26-8 CAPLUS
CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl- (6CI, 7CI) (CA INDEX NAME)



L12 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:97372 CAPLUS
DOCUMENT NUMBER: 54:97372
ORIGINAL REFERENCE NO.: 54:18423h-i,18424a-e
TITLE: Catalytic oxidation of hydrocarbons. Initiation of ozone
AUTHOR(S): Hay, Allan S.; Eustance, John W.; Blanchard, Harry S.
CORPORATE SOURCE: Gen. Elec. Research Lab., Schenectady, NY
SOURCE: Journal of Organic Chemistry (1960), 25, 616-17
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

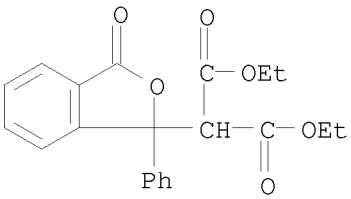
AB The isomeric xylenes were readily oxidized to the resp. toluic acids with O in AcOH at reflux temperature The reaction was catalyzed by Co ion and initiated by O3. m-Toluic acid (I) and p-toluic acid (II) were oxidized further at a slower rate to the corresponding dibasic acids. When o-toluic acid (III) was oxidized, the product, o-phthalic acid (IV), chelated with Co ion and interfered with the chain initiation step, ROOH + Co(III) → ROO• + Co(II) + H+, inhibiting the reaction. Through a mixture of 130 g. m-xylene, 40 g. Co(OAc)2.4H2O and 1 l. AcOH, 2 g./hr. O3 was passed at reflux temperature at the rate of 70 l./hr., the O3 stream stopped after 75 min., the reaction continued a further 15 hrs., the mixture cooled to room temperature, the precipitated m-C6H4(CO2H).2 (IVa) removed, an aliquot of the combined filtrate and washings evaporated to dryness, treated with dilute HCl, and extract with Et2O to give 35.2 g. I and 136.3 g. IVa. Similar results were obtained in the oxidation of p-xylene (V). o-Xylene (312 g.), 40 g.

Co(OAc)2.4H2O, and 750 ml. AcOH treated under reflux 1.5 hrs. with passage of 2.2 g./hr. O3 at a rate of 90 l./hr., at the end of 10 hrs. the mixture cooled, flooded with H2O, the precipitate filtered off and washed gave 308 g. III. No attempt was made to recover more III from the filtrate. When O3 was passed through the reaction mixture continuously, appreciable amts. of IV were formed. The following oxidns. were run with varying amts. of catalyst. An O3 (1 g./hr.) stream of 36 l./hr. passed through the solution containing the catalyst, and 10.6 g. o-xylene in 200 ml. AcOH under reflux, after 7.5 hrs. the AcOH removed, the residue treated with dilute HCl to eliminate Co salt, and I and IV separated by extraction with CHCl3. The following results were obtained [Co(OAc)2.4H2O (moles), mole yield of I and IV given]: 0.1, 0.049, 0.025; 0.02, 0.061, 0.019; 0.004, 0.061, 0.008. When O containing 1.5% O3 was passed through an AcOH solution containing 10 g. Co(OAc)2.4H2O and 20 g. IV 2 hrs. at 115°, the solution darkened slightly. The oxidation of the xylenes to phthalic acids proceeded in the presence of IV only if O3 was passed continuously during the reaction. p-Xylene (8.6 g.) and 3.3 g. IV added to 5 g. Co(OAc)2.4H2O in 200 ml. AcOH, 2 g./hr. O3 passed through 2.5 hrs. under reflux, cooled, and filtered gave 10.2 g. p-C6H4(CO2H)2 (VI). In a similar experiment 10 g. IV was added to the reaction mixture to give after 5 hrs. 9.8 g. VI. No attempt was made to isolate II. p-Methoxytoluene (12 g.) with 6 g. Co(OAc).4H2O and 200 ml. AcOH treated 1.9 hrs. with 1 g./hr. O3 under reflux, the reaction continued 2.1 hrs. further, the mixture flooded with H2O, and the product dried gave 12.2 g. p-anisic acid, m. 184-7°. Phthalide (15 g.), 5 g. Co(OAc)2.4H2O, and 300 ml. AcOH refluxed 5 hrs. with passage of 1.7 g./hr. O3 gave 13.4 g. phthalic anhydride, m. 132°.

IT 94875-82-8 111441-87-3
(Derived from data in the 6th Collective Formula Index (1957-1961))

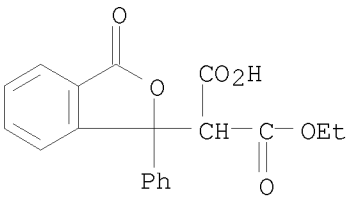
RN 94875-82-8 CAPLUS

CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)



RN 111441-87-3 CAPLUS

CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, ethyl ester (6CI) (CA INDEX NAME)



L12 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1960:44498 CAPLUS

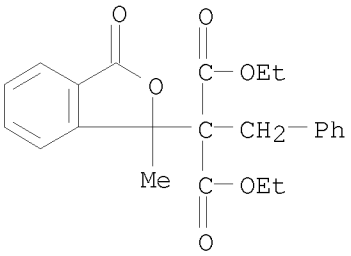
DOCUMENT NUMBER: 54:44498
ORIGINAL REFERENCE NO.: 54:8736a-b
TITLE: Ester of α-benzyl-α-[3-(3-methylphthalidyl)]malonic acid
INVENTOR(S): Matsui, Masanao; Nishizawa, Yoshihiko
PATENT ASSIGNEE(S): Sumitomo Chemical Industry Co., Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 34000960	B4	19590226	JP	<--

AB Acetophenone-o-carboxylic acid is treated with PCl5 to give 3-chloro-3-methylphthalide (I). To 0.9 g. Na in 200 cc. C6H6 is dropped 10 g. di-Et α-benzylmalonate in C6H6, the mixture heated 5 hrs., cooled, 7.3 g. I in 20 cc. C6H6 added, the mixture stirred at room temperature 1 hr., heated till the solution became neutral, cooled, and centrifuged to remove insol. matter. The supernatant fluid is concentrated and Et2O added to give 4 g. di-Et α-benzyl-α-[3-(3-methylphthalidyl)]malonate, m. 145-6° (AcOH), useful as starting material for synthesis of antibiotics, tetracycline homologs.

IT 102657-46-5P, 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 102657-46-5 CAPLUS
CN 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester (6CI) (CA INDEX NAME)



L12 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:111673 CAPLUS
DOCUMENT NUMBER: 53:111673
ORIGINAL REFERENCE NO.: 53:19985f-g
TITLE: Attempted syntheses of tetracycline analogs
AUTHOR(S): Matsui, I. Masanao; Nishizawa, Yoshihiko
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Bulletin of the Agricultural Chemical Society of Japan (1959), 23, 1-3
CODEN: BACOAV; ISSN: 0375-8397
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

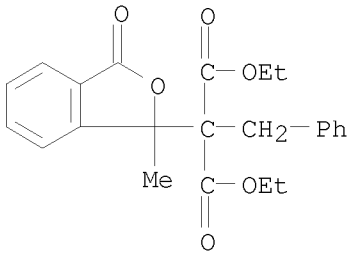
AB Several new compds. were synthesized during a series of expts. to synthesize analogs of aureomycinic acid. 3-Chloro-3-methylphthalide (I), synthesized from PCl3 and o-AcC6H4CO2H, very unstable, decompose

45°. Di-Et α-benzyl-α-[3-(3-methylphthalidyl)]malonate (II), (4 g.) prepared by refluxing 10 g. PhCH2CH(CO2Et)2 in C6H6 with 0.9 g. Na sand and adding 3 g. I, m. 141-3°. Di-Et α-benzoyl-α-[3-(3-methylphthalidyl)]succinate, (3.2 g.) prepared from 0.5 g. Na sand, 6.1 g. di-Et α-benzoylsuccinate, and 4.1 g. I in the same way as for II, m. 220-1°. 2,10-Dibromo-1,4-dioxo-1,4,5,8,9,10-hexahydronaphthalene was prepared (5.3 g.) from 4.5 g. 2,5-dibromo-p-benzoquinone and 1.6 g. butadiene by shaking in a shielded tube with 40 ml. C6H6 at 100° 6 hrs., m. 94-5°.

IT 102657-46-5P, 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 102657-46-5 CAPLUS

CN 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester (6CI) (CA INDEX NAME)



L12 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:40507 CAPLUS

DOCUMENT NUMBER: 52:40507

ORIGINAL REFERENCE NO.: 52:7266h-i,7267a-d

TITLE: Synthesis of analogs of phthalidyl degradation products of Aureomycin

AUTHOR(S): Chian, Min-Chien; Lee, Kwang-Liang; Lee, Kwang-Nien; Jen, Hsin-Min

SOURCE: Huaxue Xuebao (1956), 22, 264-70
CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal

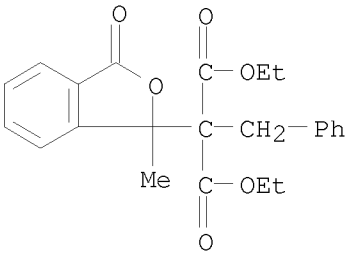
LANGUAGE: Unavailable

AB For the purpose of synthesis of de(dimethylamino)aureomycinic acid, one of the main degradation products of aureomycin, some close analogs were first prepared 3,5-R2C6H3CH2CH(CO2Et)2 (I, R = H) (Ia) were prepared from CH2(CO2Et) and the corresponding BzH followed by catalytic hydrogenation of the intermediate. I (R = OMe) (Ib) b0.1 150-5°. 2,3,6-AcXYC6H2COCl (II, X = Y = H) (IIa) m. 53-7°. Mg is dissolved in absolute MeOH to obtain Mg(OMe)2 which reacts with 5.2 g. Ia in 20 ml. benzene by stirring at 0° for 2 hrs. and separating from the solvent by centrifuging. The diethyl magnesiobenzylmalonate thus obtained reacts with IIa in C6H6 by stirring in the absence of moisture for 12, hrs. to give 6.1 g. crude III (R = X = Y = H) (IIIa), m. 106-7° (EtOH). IIa (0.75 g.) gave 0.59 g. III (R = OMe, X = Y = H) (IIIb), m. 90-1°. Both IIIa and IIIb failed to form hydrazones. Hydrolysis of IIIa and IIIb in both acidic and alkaline media by refluxing 0.2 g. with 15 ml. concentrated HCl for 36 hrs., with 7.5 ml. concentrated HCl and 7.5 ml. AcOH for 24 hrs., with 6N H2SO4 for 24 hrs., with 20 ml. fuming HCl in a sealed tube at 150-70° for 8 hrs., or with 20 ml. concentrated NH4OH, or excess Ba(OH)2-MeOH for 4 hrs. gave

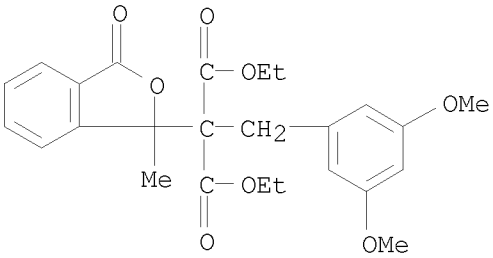
the original substances in all cases. However, IIIa and IIIb were cleaved on warming with N NaOH or KOH for 2 hrs. or on stirring at 60-70° for 4 hrs. o-AcC6H4CO2H was isolated from IIIa by acidifying and extracting with Et2O, m. 114-15°. 3-Methyl-3-hydroxy-4-chloro-7-methoxyphthalide was prepared by nitration of MeCOPh to m-O2NC6H4COMe followed by conversion of the NO2 group to the MeO group, nitration once again at 20-5° with HNO3, conversion of this NO2 group to CO2H, and chlorination.

IT 102657-46-5P, 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester 103169-80-8P, 1-Phthalanmalonic acid, α-3,5-dimethoxybenzyl-1-methyl-3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 102657-46-5 CAPLUS
CN 1-Phthalanmalonic acid, α-benzyl-1-methyl-3-oxo-, diethyl ester (6CI) (CA INDEX NAME)



RN 103169-80-8 CAPLUS
CN 1-Phthalanmalonic acid, α-3,5-dimethoxybenzyl-1-methyl-3-oxo-, diethyl ester (6CI) (CA INDEX NAME)



L12 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1956:73744 CAPLUS
DOCUMENT NUMBER: 50:73744
ORIGINAL REFERENCE NO.: 50:13810e-g
TITLE: Condensation of o-aldehydobenzoic acid and its methyl ester with malonic ester
AUTHOR(S): Rodinov, V. M.; Chukhina, E. I.
CORPORATE SOURCE: I. V. Stalin 2nd Med. Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1956), 26, 143-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

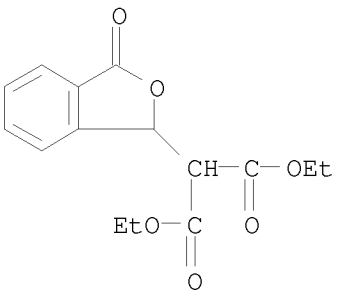
AB o-OHCC6H4CO2H (I) (11 g.), 11.73 g. CH2(CO2Et)2, and 20 ml. 12% EtOH-NH3 heated 5 hrs. on steam bath gave on treatment with Et2O 1.85 g. insol.

diphthalidylamine, m. 200-1°. This, treated with 10% H_2SO_4 and $NaNO_2$ with cooling gave I. The mother liquor from the above precipitate gave di-Et phthalidylimalonate, m. 89-90°. Heating I with $CH_2(CO_2Et)_2$ in absolute EtOH with a little piperidine gave the ψ-ester of I. Heating I with $CH_2(CO_2Et)_2$ in the presence of pyridine 10 hrs. at 107-15° gave after treatment with aqueous HCl o-$HO_2CC_6H_4CH{:}C(CO_2Et)_2$ (II), m. 39-40°; which heated with 5% alc. KOH and acidified gave o-$HO_2CC_6H_4CH{:}CHCO_2H$; the same formed on heating with EtONa. If this ester is heated with alc. NH_3 as described above, the product is di-Et phthalidylmalonate. Heating the Me ester of I with $CH_2(CO_2Et)_2$ in the presence of pyridine 10 hrs. at 115° gave a low yield of the Me ester of II, b8 235-7°, and considerable yield of II. II Me ester with aqueous Na_2CO_3 readily gave II; II Me ester in 2 months with concentrated NH_4OH gave a moderate yield of o-$H_2NCOC_6H_4CH{:}C(CONH_2)CO_2Et$, does not m. 300°. II forms only from the aldehyde-acid form of II; the phthalidylmalonic ester can form from either the aldehyde-acid form or the hydroxyphthalide form.

IT 7137-24-8P, 1-Phthalanmalonic acid, 3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 7137-24-8 CAPLUS

CN Propanedioic acid, (1,3-dihydro-3-oxo-1-isobenzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:73743 CAPLUS
DOCUMENT NUMBER: 50:73743
ORIGINAL REFERENCE NO.: 50:13810e-g
TITLE: Condensation of o-aldehydobenzoic acid and its methyl ester with malonic ester
AUTHOR(S): Rodinov, V. M.; Chukhina, E. I.
CORPORATE SOURCE: I. V. Stalin 2nd Med. Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1956), 26, 142-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

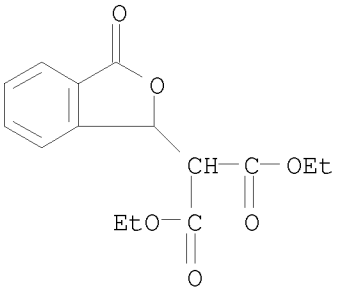
AB o-$OHCC_6H_4CO_2H$ (I) (11 g.), 11.73 g. $CH_2(CO_2Et)_2$, and 20 mL. 12% EtOH-NH_3 heated 5 h. on steam bath gave on treatment with Et_2O 1.85 g. insol. diphthalidylamine, m. 200-1°. This, treated with 10% H_2SO_4 and $NaNO_2$ with cooling gave I. The mother liquor from the above precipitate gave di-Et phthalidylimalonate, m. 89-90°. Heating I with $CH_2(CO_2Et)_2$ in absolute EtOH with a little piperidine gave the ψ-ester of I. Heating I with $CH_2(CO_2Et)_2$ in the presence of pyridine 10 h. at 107-15° gave after treatment with aqueous HCl o-$HO_2CC_6H_4CH{:}C(CO_2Et)_2$ (II), m. 39-40°; which heated with 5% alc. KOH and acidified gave

o-HO2CC6H4CH:CHCO2H; the same formed on heating with EtONa. If this ester is heated with alc. NH3 as described above, the product is di-Et phthalidylmalonate. Heating the Me ester of I with CH2(CO2Et)2 in the presence of pyridine 10 h. at 115° gave a low yield of the Me ester of II, b8 235-7°, and considerable yield of II. II Me ester with aqueous Na2CO3 readily gave II; II Me ester in 2 mo with concentrated NH4OH gave a moderate yield of o-H2NCOC6H4CH:C(CONH2)CO2Et, does not m. 300°. II forms only from the aldehyde-acid form of II; the phthalidylmalonic ester can form from either the aldehyde-acid form or the hydroxyphthalide form.

IT 7137-24-8P, 1-Phthalanmalonic acid, 3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 7137-24-8 CAPLUS

CN Propanedioic acid, (1,3-dihydro-3-oxo-1-isobenzofuranyl)-, diethyl ester (9CI) (CA INDEX NAME)



L12 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1954:60562 CAPLUS
DOCUMENT NUMBER: 48:60562
ORIGINAL REFERENCE NO.: 48:10771c-g
TITLE: Phthalide compounds
INVENTOR(S): Boothe, James H.; Kushner, Samuel
PATENT ASSIGNEE(S): American Cyanamid Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2650234		19530825	US 1952-291989	19520605 <--

GI For diagram(s), see printed CA Issue.

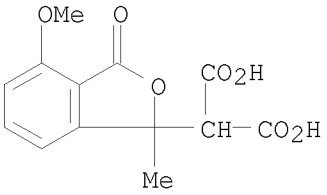
AB New carboxylic acid esters (I) have been prepared in which R represents a lower alkyl radical, R' represents either H, lower alkoxy radicals, lower alkyl radicals, or lower alkyl radicals having a carboxyl ester substituent, and R''and R''' represent esterified radicals. 3-Methyl-3-chloro-7-methoxyphthalide (II) 4 is added slowly to NaC(CO2Et)2CH2CO2Et (II) 6 parts by weight in dry C6H6 the solution refluxed, cooled, centrifuged, the supernatent liquid evaporated to dryness, and the residue of 3-methyl-3-(1,1,2-tricarbethoxyethyl)-7-methoxyphthalide recrystd. 3 times from ether. The 3-(1,1,2-tricarbomethoxyethyl) analog is prepared by substituting an equal molar quantity of NaC(CO2Me)2CH2CO2Me for III. II (4 parts by weight) is treated 3 hrs. with magnesiomalonic ester (IV) (from 5.4 parts by volume of malonic ester and 2.65 parts by weight of

Mg(OMe)2 in 35 parts by volume of dry C6H6), the mixture evaporated to dryness, 25
parts by volume of CHCl3 added, the CHCl3 layer separated, dried, evaporated to dryness, and the residue of 3-methyl-3-(dicarbethoxymethyl)-7-methoxyphthalide crystallized twice from AcOEt, then from EtOH; the 3-(dicarbomethoxymethyl) homolog is similarly prepared from the di Me ester of magnesiomalonic acid.

IT 856803-18-4, 1-Phthalanmalonic acid, 4-methoxy-1-methyl-3-oxo-
859299-05-1, Phthalide, 7-methoxy-3-methyl-3-(1,1,2-tricarboxyethyl)-
(esters)

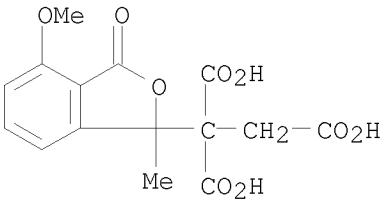
RN 856803-18-4 CAPLUS

CN Propanedioic acid, 2-(1,3-dihydro-4-methoxy-1-methyl-3-oxo-1-isobenzofuranyl)- (CA INDEX NAME)



RN 859299-05-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L12 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1954:56588 CAPLUS

DOCUMENT NUMBER: 48:56588

ORIGINAL REFERENCE NO.: 48:9971a-i

TITLE: Synthesis of degradation products of Aureomycin. V

AUTHOR(S): Boothe, J. H.; Kushner, S.; Williams, J. H.

CORPORATE SOURCE: American Cyanamid Co., Pearl River, NY

SOURCE: Journal of the American Chemical Society (1953), 75, 3263-4
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

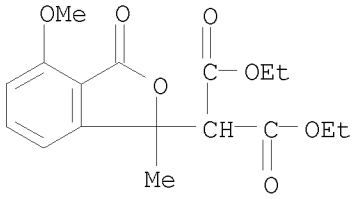
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 48:56588

AB (4-Chloro-7-methoxy-3-methylphthalidyl)succinic acid (V), a degradation product of Aureomycin, has been synthesized. The synthesis involves a new method of adding substituents to the 3-position of a phthalide by reaction of a pseudo acid chloride with a malonic ester derivative II (5 g.) and 5.6 g. PCl5 in 50 cc. dry C6H6 stirred 1 hr., the solution diluted with 150 cc. dry heptane, cooled 3 hrs., and the crystalline deposit washed with low-boiling petr. ether gave 4-4.5 g. product, which was predominantly 3-chloro-7-methoxy-3-methylphthalide (VI). CH2(CO2Et)2 (5.47 cc.) shaken 3 hrs. with 2.65 g. Mg(OMe)2.2MeOH in 35 cc. dry C6H6, the mixture

centrifuged clear, evaporated to dryness in vacuo, the residue dissolved in 25 cc. dry C6H6, the solution stirred 2 hrs. with the VI, the mixture evaporated to dryness in vacuo, the residue treated with 25 cc. H2O and 1.5 cc. concentrated HCl, extracted with CHCl3, the extract dried, evaporated to dryness, the residue mixed with petr. ether, and the resulting solid filtered off and recrystd. from 5 cc. EtOH gave 2.44 g. di-Et (7-methoxy-3-methylphthalidyl)malonate (VIa), m. 120-2°; recrystd. from EtOAc and then EtOH, it m. 125-6.5°. EtO2CCH2CH(CO2Et)2 (6 g.) and 1.39 g. NaOMe in 35 cc. dry C6H6 evaporated to dryness, the residual sirup redissolved in 35 cc. dry C6H6, treated during 20 min. with a suspension of VI (prepared from 5 g. II) in 40 cc. dry C6H6, the mixture refluxed 0.5 hr., cooled, centrifuged, the clear C6H6 solution concentrated to dryness in vacuo, and the yellow oily residue diluted with 15 cc. Et2O and cooled several hrs. gave 4.55 g. tri-Et ester (VII) of the tricarboxylic acid (VIII), m. 80-5°; recrystd. twice from Et2O, it m. 83-5°. VII (422 mg.) in 3 cc. EtOH treated during 0.5 hr. dropwise with stirring with 3.1N NaOH, and the mixture let stand 0.5 hr. and acidified slowly deposited II, m. 160-2°, also obtained by heating VII 1 hr. with N NaOH on the steam bath or by refluxing 18 hrs. with 0.5N Na2CO3. VII (0.6 g.) refluxed 1.5 hrs. with 12 cc. concentrated HCl, the nearly clear solution diluted with 20 cc. H2O, filtered, cooled, and the resulting crystalline product recrystd. from 10 cc. H2O yielded about 0.2 g. of the α-(carboxymethyl) derivative (IX) of VIa, m. 166-8°; recrystd. from 8 cc. C6H6, it m. 169-70.5°. IX (0.2 g.) let stand 3 hrs. at room temperature with 5 cc. 0.5N NaOH, and the solution diluted to 10 cc., acidified with HCl, and cooled gave II. VII (20 g.) refluxed 16 hrs. with 400 cc. concentrated HCl, the solution concentrated in vacuo to about 50 cc., cooled, the crude product (7-8 g.), m. 185-95° (decomposition), extracted 0.5 hr. with 400 cc. boiling EtOH, and the insol. residue filtered off hot gave about 2 g. (7-methoxy-3-methylphthalidyl)succinic acid (Xa), m. 204-8° (decomposition); recrystd. from H2O, it m. 207-9.5°. The EtOAc filtrate let stand 3 days deposited 2.9 g. crystalline material, m. 190° (decomposition), the filtrate from which, concentrated to 60 cc. and cooled, deposited 1.05 g. solid, m. 186-8° (decomposition); a 0.5-g. sample of this material boiled with 75 cc. EtOAc, a small amount of undissolved solid, m. 189-91° (decomposition), filtered off, and the filtrate cooled gave an isomer (Xb) of Xa, m. 190-1°. Xb (1 g.) dissolved in 50 cc. AcOH by heating, the solution cooled to 40°, let stand 3.5 hrs. with 7.2 cc. 6.6% Cl in AcOH at room temperature, concentrated to dryness in vacuo, and the residue stirred with 10 cc. C6H6 and cooled gave 530 mg. 4-Cl derivative of Xb, m. 199-200° (decomposition) (from EtOAc-petr. ether). Similarly was prepared the 4-Cl derivative (XI) of Xa, m. 228-9° (from EtOAc-petr. ether). XI (0.5 g.) in 10 cc. EtOH and 1.2 g. anhydrous brucine in 10 cc. EtOH gave 0.51 g. crude brucine salt which was recrystd. twice from EtOH to yield 0.4 g.; a 0.38-g. sample in 10 cc. H2O acidified with 5 drops concentrated HCl and extracted with four 20-cc. portions of EtOAc, the extract washed with 10 cc. H2O, dried, evaporated to dryness in vacuo, and the residue (150 mg.) clarified with Norit and recrystd. from 8 cc. H2O gave I, m. 209-10.5° (decomposition), [α]25D -20.4° (5% in EtOH). Racemic I (0.4 g.) heated 2.5 hrs. with 8 cc. Ac2O on the steam bath, the solution concentrated to dryness in vacuo, and the residue recrystd. from 45 cc. dry C6H6 gave the anhydride of I, m. 202-4°. Optically active I was converted similarly to the anhydride, m. 200-1°.

IT 856803-15-1P, 1-Phthalanmalonic acid, 4-methoxy-1-methyl-3-oxo-, diethyl ester
RL: PREP (Preparation)
(preparation of)
RN 856803-15-1 CAPLUS
CN Propanedioic acid, 2-(1,3-dihydro-4-methoxy-1-methyl-3-oxo-1-isobenzofuranyl)-, 1,3-diethyl ester (CA INDEX NAME)



L12 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1952:26770 CAPLUS
DOCUMENT NUMBER: 46:26770
ORIGINAL REFERENCE NO.: 46:4570h-i,4571a-d
TITLE: 3-Phenyl-3-phthalide-3-acetic acid
INVENTOR(S): Burger, Alfred
PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2567546		19510911	US 1950-178343	19500808 <--

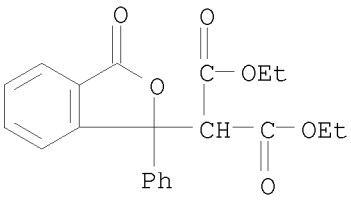
AB The preparation of 3-phenyl-3-phthalideacetic acid (I), a useful pharmaceutical intermediate, is described. o-BzC6H4CO2H (II) 33.9 g. in 280 cc. anhydrous Et2O is added to a suspension of CH2:CH2CH2MgCl (from 24.3 g. Mg in 500 cc. dry Et2O to which 38.5 g. CH2: CHCH2Cl in 450 cc. dry Et2O is added at a rate of 2 cc./min. and the mixture stirred and refluxed 15 min.) over 1.25 hrs. while the solvent is distilled at the same rate; when the addition is complete 930 cc. C6H6 is added, distillation continued until the liquid temperature is 80°, the solution refluxed 11 hrs., the Grignard complex decomposed with 100 cc. ice water and, after decantation from the excess Mg, with 500 cc. 9% HCl, the organic layer separated, washed with H2O, then with NaHCO3 until neutral, dried, the solvent removed, and the residue distilled giving 3-allyl-3-phenylphthalide (III), b1 180-6°, nD25 1.5797; the redistd. III b. 153-4° nD25 1.5848. III 1 and KMnO4 1.7 g. in 20 ml. H2O are refluxed 35 min., the solution filtered and acidified with concentrated HCl, and the oil extracted with C6H6, dried, and evaporated; addition of CHCl3 to the residue ppts. I, m. 173-5°. II 45.2 and SOCl2 95.2 g. are warmed 20 hrs. at 50° while dry preheated (50°) air is passed over the surface, then bubbled 5 hrs. through the solution until the excess SOCl2 is removed, to give the pseudo acid chloride of I. This is added rapidly in 100 cc. dry Et2O with good stirring to EtOMgCH(CO2Et)2, forming a pale green sirup, which is refluxed 1 hr., allowed to stand overnight, decomposed with ice cold 37% H2SO4, the mixture extracted with Et2O and NaHCO3

(10%), washed with H2O, and the C6H6 removed, leaving an oily residue; addition of absolute Et2O ppts. di-Et 3-phenyl-3-phthalidemalonate (IV), m. 77-9°. IV, 2.5 g. in 10 cc. absolute EtOH refluxed 1 hr. with 10 cc. 40% KOH, the mixture diluted portionwise with H2O, 30 cc. of a mixture of EtOH and H2O distilled off, the residue extracted with C6H6, the alkaline layer acidified with HCl, extracted with C6H6, and the extract dried and evaporated ppts. microcryst. material which, after washing with CHCl3 and drying, gives I, m. 175-7°. I 8 g. is refluxed 1 hr. with 15 cc. SOCl2, the excess SOCl2 removed in vacuo, the residue refluxed 2 hrs. in 75 cc. dry C6H6 with 7 g. Et2NCH2CH2NH2, and the mixture cooled and washed twice with 25 cc. NaHCO3 solution and H2O until neutral, yielding N-(2-diethylaminoethyl)-3-phenyl-3-phthalideacetamide, m. 129-9.5°.

IT 94875-82-8P, 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 94875-82-8 CAPLUS

CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)



L12 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1951:16487 CAPLUS
DOCUMENT NUMBER: 45:16487
ORIGINAL REFERENCE NO.: 45:2928i,2929a-g
TITLE: Rearrangement of diethyl 3-phenylphthalidyl-3-malonate to derivatives of 3-phenylindone-2-carboxylic acid
AUTHOR(S): Yost, Wm. L.; Burger, Alfred
CORPORATE SOURCE: Univ. of Virginia, Charlottesville
SOURCE: Journal of Organic Chemistry (1950), 15, 1113-18
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 45:16487

GI For diagram(s), see printed CA Issue.

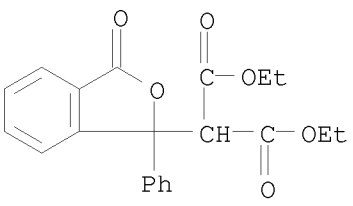
AB Because the lactone ring in phthalein indicators is extremely sensitive to dilute alkali, whereas 3,3-diphenyl- and certain 3,3-dialkylphthalides are stable to acid and bases, a number of 3-alkyl-3-arylphthalides are prepared and the effect of various functional groups in the alkyl group on the stability of the furanone ring is studied. A stream of dried air is passed 20 hrs. over the surface of a mixture of 45.2 g. o-BzC6H4CO2H (I) and 95.2 g. SOCl2 at 50°, then dry air is passed 5 hrs. through the mixture, and the cooled sirupy residue dissolved in 100 cc. ether and added rapidly with stirring to Mg[CH(CO2Et)2]2 from 35.2 g. ester, giving a thick, sirupy, greenish precipitate The mixture is stirred 1 hr., kept overnight, cooled, and decomposed with 130 cc. 37% H2SO4, the ether solution washed with H2O, extracted with 10% Na2CO3 and H2O, the residue dried by

distilling it with C6H6 to near dryness, and absolute ether added, giving 24% di-Et 3-phenyl-3-phthalidemalonate (II), crystals from absolute ether, m. 77-9°. Acidification of the washed (ether) Na2CO3 exts. gives a small amount of Et 3-phenylindone-2-carboxylate (III), highly refractive deep yellow crystals, m. 86-7.5°. Distillation of the residue of the ether mother liquors of II in vacuo gives 23.4% III. Warming 10 g. II in 100 cc. 10% Na2CO3 20 min. at 50° and neutralizing the clear solution with 6 N HCl give 88.8% III. Heating 3.68 g. II 1 hr. in 10 cc. AcOH containing 1 cc. H2O and 5 drops concentrated H2SO4 while distilling off the AcOEt formed, diluting the mixture with 20 cc. H2O, extracting it with C6H6, extracting the H2O-washed C6H6 solution with 10% Na2CO3, and acidifying the alkaline solution with 6 N HCl give 100% 3-phenylindone-2-carboxylic acid (IV), brilliant red felted needles, m. 153.5-6°. Hydrogenation of 1.8 g. III in 25 cc. absolute EtOH with Raney Ni at 34° gives crude Et 1-oxo-3-phenyl-2-indancarboxylate, m. 86-7.5°, which, hydrolyzed 1 hr. at 90° with 10 cc. AcOH containing a trace of 50% H2SO4, gives 3-phenyl-1-indanone (V) (semicarbazone, m. 217.5-19.5°). Hydrogenation of 1.28 g. IV in 25 cc. absolute EtOH in the presence of PdCl4 at 34° gives V. Gently refluxing 2.5 g. II 1 hr. in 10 cc. EtOH and 10 cc. 40% KOH, distilling off 30 cc. alc. with simultaneous addition of 30 cc. H2O, extracting the mixture with C6H6, acidifying the alkaline solution with concentrated HCl, extracting it with C6H6, evaporating the dried extract, and treating the residue with CHCl3 give 3-phenyl-3-phthalideacetic acid, o-C6H4.CO.O.CPhCH2CO2H, m. 175-7°, which is also obtained by refluxing 1 g. 3-allyl-3-phenylphthalide (VI) with 1.7 g. KMnO4 in 20 cc. H2O 35 min. and acidifying the filtered solution with concentrated HCl. Addition of 33.9 g. I in 280 cc. ether over a period of 1.25 hrs. to CH2:CHCH2MgBr from 38.5 g. bromide in 950 cc. ether while simultaneously distilling off ether at the same rate, adding 930 cc. C6H6, distilling off the ether until the temperature of the mixture reaches 80°, refluxing the latter 11 hrs., hydrolyzing it with 100 cc. ice H2O, decanting the liquid from the excess Mg, treating the residue with 300 cc. 9% HCl, and distilling the residue of the washed (H2O, NaHCO3, H2O) and dried C6H6 layer give 57.1% VI, b0.4 168-9.5°, n25D 1.5808, b0.2 153-4°, n25D 1.5848.

IT 94875-82-8, 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (and rearrangement thereof)

RN 94875-82-8 CAPLUS

CN 1-Phthalanmalonic acid, 3-oxo-1-phenyl-, diethyl ester (6CI, 7CI) (CA INDEX NAME)



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L3             8 S L1
L4           133 S L1 FULL

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L12           53 L11 NOT L6

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